

Figure 1: HIV-1 gp41 Structure and Peptides

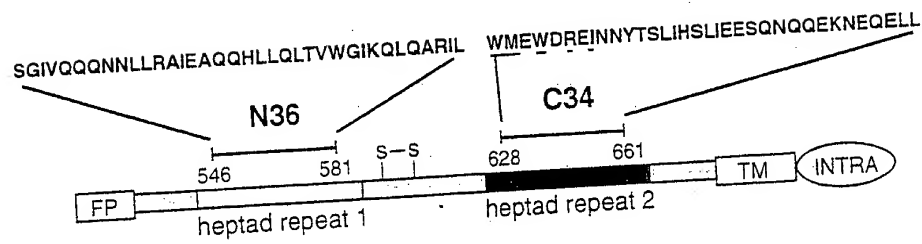
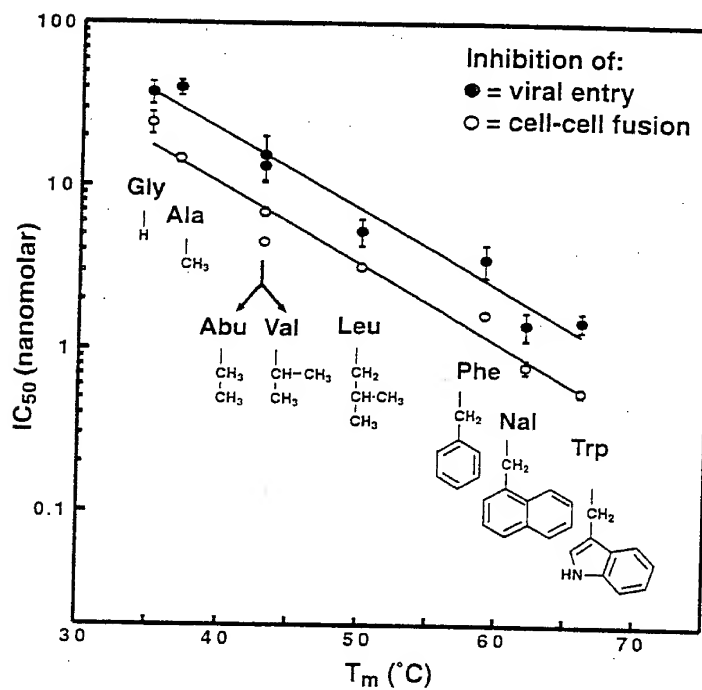


Figure 2: Correlation of C34 Inhibitory Potency With N36/C34 Stability



001221-21234260

Figure 3: D-peptide Sequences

D10pep1 : Ac- G A C E A R H R E W A W L C A A - CONH2
D10pep1a: Ac - K K G A C E A R H R E W A W L C A A - CONH2
D10pep3 : Ac - K K G A C G L G Q E E W F W L C A A - CONH2
D10pep4 : Ac - G A C D L K A K E W F W L C A A - CONH2
D10pep5 : Ac - K K G A C E L L G W E W A W L C A A - CONH2
D10pep5a: Ac - K K K K G A C E L L G W E W A W L C A A - CONH2
D10pep6 : Ac - G A C S R S Q P E W E W L C A A - CONH2
D10pep6a: Ac - K K G A C S R S Q P E W E W L C A A - CONH2
D10pep7a: Ac - K K G A C L L R A P E W G W L C A A - CONH2
D10pep10: Ac - K K G A C M R G E W E W S W L C A A - CONH2
D10pep12: Ac - K K G A C P P L N K E W A W L C A A - CONH2
Consensus Sequence C X X X X X E W X W L C

Where:

G = glycine
A = alanine
C = cysteine
D = aspartic acid
L = leucine
K = lysine
E = glutamic acid
W = tryptophan
F = phenylalanine
R = arginine
H = histidine
S = serine
Q = glutamine

00745713-132400

Figure 4: Mirror-Image Phage Display with the D-IQN17 Target

1. Perform rounds of phage selection to identify binders to D-IQN17.

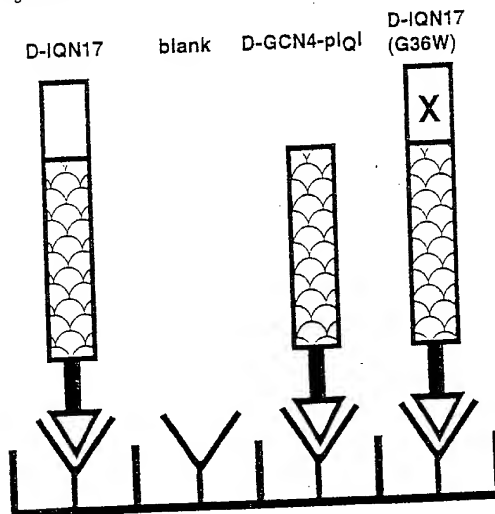
D-IQN17



Phage Library:
C/SXXXXXXXXXXC/S

← linker with trypsin site
← biotin

2. Sequence individual phage clones
3. Test for specificity of binding. Determine if the phage bind to the gp41 region of D-IQN17.



4. Synthesize D-peptides.
5. Assay anti-HIV activity of D-peptides.

Relationship of D-peptides to IQN17

Figure 5A

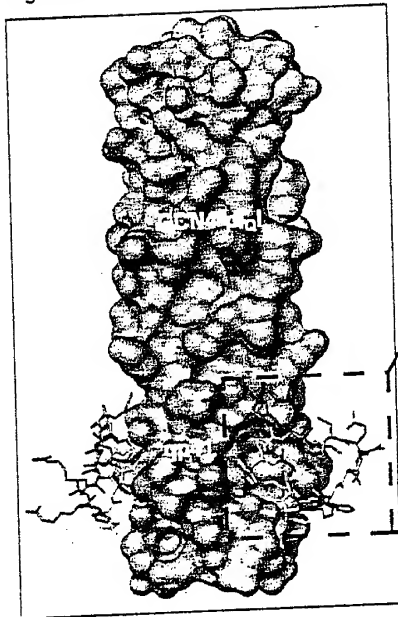
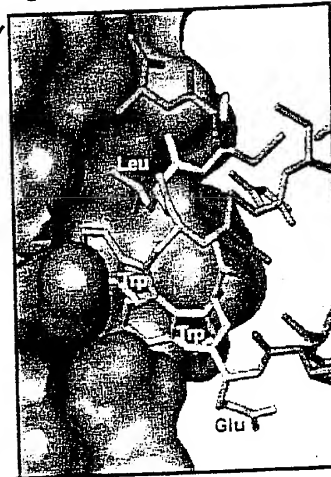


Figure 5B



00745742.122400

Syncytia Assays

Figure 6A

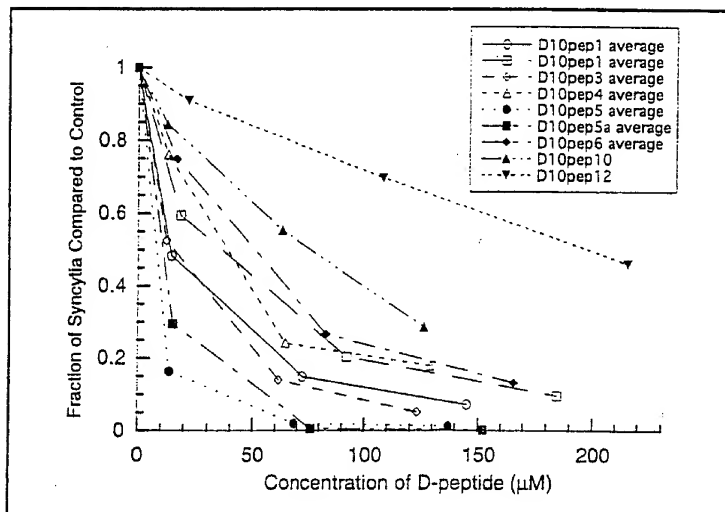


Figure 6B: IC₅₀ Data for D-Peptides:

D-Peptide	Approximate IC ₅₀ Value (from one or more experiments)
D10pep1	2×10^{-5} M
D10pep1A	3×10^{-5} M
D10pep3	1×10^{-5} M
D10pep4	3×10^{-5} M
D10pep5	3×10^{-6} M
D10pep5a	6×10^{-6} M
D10pep6	3×10^{-5} M
D10pep7a	4×10^{-5} M
Dpep10	6×10^{-5} M
Dpep12	2×10^{-4} M

D10pep3 } show anti-viral effects
 D10pep4 } with IC₅₀ values of
 D10pep5 } less than 1×10^{-4} M.

REMARK 3
 REMARK 3 REFINEMENT
 REMARK 3 PROGRAM : CNS 0.5
 REMARK 3 AUTHORS : BRUNGER, ADAMS, CLORE, DELANO,
 REMARK 3 GROS, GROSSE-KUNSTLEVE, JIANG,
 REMARK 3 KUSZEWSKI, NILGES, PANNU, READ,
 REMARK 3 RICE, SIMONSON, WARREN
 REMARK 3
 REMARK 3 DATA USED IN REFINEMENT.
 REMARK 3 RESOLUTION RANGE HIGH (ANGSTROMS) : 1.50
 REMARK 3 RESOLUTION RANGE LOW (ANGSTROMS) : 10.00
 REMARK 3 (SIGMA(F)) : 0.0
 REMARK 3 DATA CUTOFF (ABS(F)) : 646169.44
 REMARK 3 DATA CUTOFF HIGH (ABS(F)) : 0.000000
 REMARK 3 DATA CUTOFF LOW (ABS(F)) : 0.000000
 REMARK 3 COMPLETENESS (WORKING+TEST) (%) : 94.6
 REMARK 3 NUMBER OF REFLECTIONS : 13549
 REMARK 3
 REMARK 3 FIT TO DATA USED IN REFINEMENT.
 REMARK 3 CROSS-VALIDATION METHOD : THROUGHOUT
 REMARK 3 FREE R VALUE TEST SET SELECTION : RANDOM
 REMARK 3 R VALUE (WORKING SET) : 0.214
 REMARK 3 FREE R VALUE : 0.245
 REMARK 3 FREE R VALUE TEST SET SIZE (%) : 10.1
 REMARK 3 FREE R VALUE TEST SET COUNT : 1362
 REMARK 3 ESTIMATED ERROR OF FREE R VALUE : 0.007
 REMARK 3
 REMARK 3 FIT IN THE HIGHEST RESOLUTION BIN.
 REMARK 3 TOTAL NUMBER OF BINS USED : 6
 REMARK 3 BIN RESOLUTION RANGE HIGH (A) : 1.50
 REMARK 3 BIN RESOLUTION RANGE LOW (A) : 1.59
 REMARK 3 BIN COMPLETENESS (WORKING+TEST) (%) : 96.1
 REMARK 3 REFLECTIONS IN BIN (WORKING SET) : 2008
 REMARK 3 BIN R VALUE (WORKING SET) : 0.233
 REMARK 3 BIN FREE R VALUE : 0.270
 REMARK 3 BIN FREE R VALUE TEST SET SIZE (%) : 9.8
 REMARK 3 BIN FREE R VALUE TEST SET COUNT : 219
 REMARK 3 ESTIMATED ERROR OF BIN FREE R VALUE : 0.018
 REMARK 3
 REMARK 3 NUMBER OF NON-HYDROGEN ATOMS USED IN REFINEMENT.
 REMARK 3 PROTEIN ATOMS : 0
 REMARK 3 NUCLEIC ACID ATOMS : 0
 REMARK 3 HETEROGEN ATOMS : 0
 REMARK 3 SOLVENT ATOMS : 0
 REMARK 3
 REMARK 3 B VALUES.
 REMARK 3 FROM WILSON PLOT (A**2) : 21.6
 REMARK 3 MEAN B VALUE (OVERALL, A**2) : 29.7
 REMARK 3 OVERALL ANISOTROPIC B VALUE.
 REMARK 3 B11 (A**2) : 3.61
 REMARK 3 B22 (A**2) : 3.61
 REMARK 3 B33 (A**2) : -7.22
 REMARK 3 B12 (A**2) : 1.74
 REMARK 3 B13 (A**2) : 0.00
 REMARK 3 B23 (A**2) : 0.00
 REMARK 3
 REMARK 3 BULK SOLVENT MODELING.
 REMARK 3 METHOD USED : FLAT MODEL
 REMARK 3 KSOL : 0.194054

Figure 7A

Figure 7B

Figure 7C

ATOM	54	OE1	GLU	A	6	23.016	3.931	-16.557	1.00	52.29	A
ATOM	55	OE2	GLU	A	6	21.019	4.682	-17.116	1.00	52.25	A
ATOM	56	C	GLU	A	6	23.995	5.606	-11.904	1.00	49.32	A
ATOM	57	O	GLU	A	6	23.475	5.210	-10.859	1.00	49.24	A
ATOM	58	N	ASP	A	7	25.302	5.527	-12.128	1.00	48.32	A
ATOM	59	CA	ASP	A	7	26.178	4.970	-11.113	1.00	47.23	A
ATOM	60	CB	ASP	A	7	27.543	4.626	-11.703	1.00	47.92	A
ATOM	61	CG	ASP	A	7	27.450	3.585	-12.788	1.00	48.33	A
ATOM	62	OD1	ASP	A	7	26.526	2.741	-12.729	1.00	48.43	A
ATOM	63	OD2	ASP	A	7	28.310	3.606	-13.690	1.00	48.94	A
ATOM	64	C	ASP	A	7	26.344	5.920	-9.926	1.00	46.09	A
ATOM	65	O	ASP	A	7	26.283	5.481	-8.773	1.00	45.71	A
ATOM	66	N	LYS	A	8	26.551	7.209	-10.201	1.00	44.57	A
ATOM	67	CA	LYS	A	8	26.703	8.195	-9.129	1.00	43.01	A
ATOM	68	CB	LYS	A	8	26.959	9.598	-9.708	1.00	43.49	A
ATOM	69	CG	LYS	A	8	25.895	10.076	-10.695	1.00	44.78	A
ATOM	70	CD	LYS	A	8	26.423	11.125	-11.702	1.00	45.38	A
ATOM	71	CE	LYS	A	8	26.698	12.490	-11.068	1.00	45.64	A
ATOM	72	NZ	LYS	A	8	27.153	13.499	-12.069	1.00	45.55	A
ATOM	73	C	LYS	A	8	25.413	8.171	-8.318	1.00	41.20	A
ATOM	74	O	LYS	A	8	25.419	8.346	-7.098	1.00	40.61	A
ATOM	75	N	ILE	A	9	24.302	7.935	-9.002	1.00	39.40	A
ATOM	76	CA	ILE	A	9	23.015	7.859	-8.333	1.00	37.29	A
ATOM	77	CB	ILE	A	9	21.872	7.859	-9.358	1.00	37.14	A
ATOM	78	CG2	ILE	A	9	20.600	7.251	-8.759	1.00	37.06	A
ATOM	79	GD1	ILE	A	9	21.631	9.303	-9.812	1.00	36.95	A
ATOM	80	CD1	ILE	A	9	20.801	9.440	-11.066	1.00	36.89	A
ATOM	81	C	ILE	A	9	22.927	6.638	-7.418	1.00	36.07	A
ATOM	82	O	ILE	A	9	22.450	6.756	-6.292	1.00	34.70	A
ATOM	83	N	GLU	A	10	23.389	5.478	-7.887	1.00	34.23	A
ATOM	84	CA	GLU	A	10	23.353	4.260	-7.074	1.00	33.04	A
ATOM	85	CB	GLU	A	10	23.884	3.013	-7.847	1.00	32.87	A
ATOM	86	CG	GLU	A	10	23.890	1.705	-6.991	1.00	33.10	A
ATOM	87	CD	GLU	A	10	24.287	0.417	-7.747	1.00	33.56	A
ATOM	88	OE1	GLU	A	10	24.327	0.442	-8.999	1.00	34.07	A
ATOM	89	OE2	GLU	A	10	24.542	-0.630	-7.084	1.00	32.41	A
ATOM	90	C	GLU	A	10	24.244	4.556	-5.878	1.00	32.53	A
ATOM	91	O	GLU	A	10	24.009	4.069	-4.779	1.00	32.14	A
ATOM	92	N	GLU	A	11	25.259	5.380	-6.100	1.00	31.82	A
ATOM	93	CA	GLU	A	11	26.165	5.731	-5.018	1.00	31.36	A
ATOM	94	CB	GLU	A	11	27.409	6.445	-5.536	1.00	33.18	A
ATOM	95	CG	GLU	A	11	28.358	6.833	-4.423	1.00	35.22	A
ATOM	96	CD	GLU	A	11	29.105					

Figure 7D

ATOM	112	CG	GLU	A	13	19.760	5.937	-4.810	1.00	29.72	A
ATOM	113	CD	GLU	A	13	19.080	5.118	-5.900	1.00	31.77	A
ATOM	114	OE1	GLU	A	13	19.671	4.107	-6.331	1.00	33.64	A
ATOM	115	OE2	GLU	A	13	17.960	5.495	-6.327	1.00	32.24	A
ATOM	116	C	GLU	A	13	21.975	5.110	-1.678	1.00	26.36	A
ATOM	117	O	GLU	A	13	21.411	4.912	-0.597	1.00	25.75	A
ATOM	118	N	SER	A	14	23.179	4.629	-1.950	1.00	26.17	A
ATOM	119	CA	SER	A	14	23.899	3.792	-0.999	1.00	26.31	A
ATOM	120	CB	SER	A	14	25.184	3.224	-1.625	1.00	26.71	A
ATOM	121	OG	SER	A	14	25.954	2.470	-0.695	1.00	30.07	A
ATOM	122	C	SER	A	14	24.246	4.626	0.221	1.00	25.81	A
ATOM	123	O	SER	A	14	24.079	4.149	1.339	1.00	25.13	A
ATOM	124	N	LYS	A	15	24.753	5.840	0.009	1.00	24.70	A
ATOM	125	CA	LYS	A	15	25.091	6.713	1.151	1.00	25.41	A
ATOM	126	CB	LYS	A	15	25.805	7.971	0.672	1.00	26.20	A
ATOM	127	CG	LYS	A	15	27.256	7.762	0.285	1.00	29.07	A
ATOM	128	CD	LYS	A	15	27.875	9.077	-0.220	1.00	30.97	A
ATOM	129	CE	LYS	A	15	29.328	8.914	-0.603	1.00	32.08	A
ATOM	130	NZ	LYS	A	15	29.547	7.749	-1.502	1.00	34.63	A
ATOM	131	C	LYS	A	15	23.824	7.102	1.938	1.00	24.45	A
ATOM	132	O	LYS	A	15	23.862	7.279	3.171	1.00	24.50	A
ATOM	133	N	GLN	A	16	22.708	7.254	1.247	1.00	24.12	A
ATOM	134	CA	GLN	A	16	21.450	7.586	1.904	1.00	23.82	A
ATOM	135	CB	GLN	A	16	20.396	7.815	0.834	1.00	25.71	A
ATOM	136	CG	GLN	A	16	19.229	8.643	1.232	1.00	29.64	A
ATOM	137	CD	GLN	A	16	18.543	9.230	0.004	1.00	32.26	A
ATOM	138	OE1	GLN	A	16	18.015	8.498	-0.817	1.00	34.89	A
ATOM	139	NE2	GLN	A	16	18.569	10.556	-0.135	1.00	32.74	A
ATOM	140	C	GLN	A	16	21.027	6.447	2.838	1.00	23.67	A
ATOM	141	O	GLN	A	16	20.584	6.681	3.979	1.00	22.84	A
ATOM	142	N	LYS	A	17	21.160	5.214	2.365	1.00	22.83	A
ATOM	143	CA	LYS	A	17	20.798	4.057	3.179	1.00	22.59	A
ATOM	144	CB	LYS	A	17	20.939	2.756	2.357	1.00	22.86	A
ATOM	145	CG	LYS	A	17	20.340	1.539	3.055	1.00	26.69	A
ATOM	146	CD	LYS	A	17	18.837	1.579	2.932	1.00	29.27	A
ATOM	147	CE	LYS	A	17	18.177	0.937	4.051	1.00	31.75	A
ATOM	148	NZ	LYS	A	17	16.686	0.870	3.940	1.00	34.25	A
ATOM	149	C	LYS	A	17	21.718	4.015	4.406	1.00	22.31	A
ATOM	150	O	LYS	A	17	21.261	3.747	5.515	1.00	21.02	A
ATOM	151	N	LYS	A	18	23.001	4.306	4.223	1.00	21.81	A
ATOM	152	CA	LYS	A	18	23.909	4.302	5.374	1.00	21.74	A
ATOM	153	CB	LYS	A	18	2					

Figure 7E

ATOM	170	CB	GLU	A	20	18.223	5.608	6.484	1.00	22.94	A
ATOM	171	CG	GLU	A	20	17.766	6.671	5.499	1.00	25.51	A
ATOM	172	CD	GLU	A	20	16.926	6.108	4.378	1.00	29.04	A
ATOM	173	OE1	GLU	A	20	16.961	4.873	4.177	1.00	30.40	A
ATOM	174	OE2	GLU	A	20	16.243	6.901	3.691	1.00	30.73	A
ATOM	175	C	GLU	A	20	19.533	5.109	8.576	1.00	20.88	A
ATOM	176	O	GLU	A	20	18.917	5.127	9.645	1.00	20.22	A
ATOM	177	N	ASN	A	21	20.478	4.220	8.321	1.00	20.53	A
ATOM	178	CA	ASN	A	21	20.820	3.212	9.328	1.00	21.87	A
ATOM	179	CB	ASN	A	21	21.694	2.117	8.720	1.00	24.15	A
ATOM	180	CG	ASN	A	21	20.875	1.155	7.872	1.00	25.28	A
ATOM	181	OD1	ASN	A	21	19.676	0.980	8.099	1.00	28.26	A
ATOM	182	ND2	ASN	A	21	21.505	0.549	6.870	1.00	26.78	A
ATOM	183	C	ASN	A	21	21.500	3.854	10.527	1.00	21.75	A
ATOM	184	O	ASN	A	21	21.269	2.444	11.674	1.00	21.80	A
ATOM	185	N	GLU	A	22	22.335	4.853	10.274	1.00	20.99	A
ATOM	186	CA	GLU	A	22	23.007	5.548	11.369	1.00	20.36	A
ATOM	187	CB	GLU	A	22	24.059	6.516	10.825	1.00	22.89	A
ATOM	188	CG	GLU	A	22	24.914	7.169	11.901	1.00	25.86	A
ATOM	189	CD	GLU	A	22	25.515	6.170	12.444	1.00	27.97	A
ATOM	190	OE1	GLU	A	22	26.121	5.158	12.882	1.00	30.05	A
ATOM	191	OE2	GLU	A	22	25.376	6.411	14.118	1.00	31.29	A
ATOM	192	C	GLU	A	22	21.952	6.294	12.187	1.00	19.79	A
ATOM	193	O	GLU	A	22	21.988	6.264	13.445	1.00	18.87	A
ATOM	194	N	ILE	A	23	21.003	6.951	11.518	1.00	18.92	A
ATOM	195	CA	ILE	A	23	19.955	7.670	12.254	1.00	18.60	A
ATOM	196	CB	ILE	A	23	19.012	8.388	11.244	1.00	18.79	A
ATOM	197	CG2	ILE	A	23	17.672	8.764	11.880	1.00	20.11	A
ATOM	198	CG1	ILE	A	23	19.739	9.598	10.701	1.00	20.45	A
ATOM	199	CD1	ILE	A	23	19.060	10.223	9.539	1.00	22.51	A
ATOM	200	C	ILE	A	23	19.163	6.687	13.118	1.00	19.09	A
ATOM	201	O	ILE	A	23	18.807	7.006	14.260	1.00	18.74	A
ATOM	202	N	ALA	A	24	18.903	5.479	12.617	1.00	18.44	A
ATOM	203	CA	ALA	A	24	18.153	4.517	13.420	1.00	18.86	A
ATOM	204	CB	ALA	A	24	17.824	3.257	12.573	1.00	19.39	A
ATOM	205	C	ALA	A	24	18.947	4.136	14.665	1.00	18.66	A
ATOM	206	O	ALA	A	24	18.343	3.966	15.757	1.00	19.32	A
ATOM	207	N	ARG	A	25	20.272	4.028	14.548	1.00	18.57	A
ATOM	208	CA	ARG	A	25	21.111	3.667	15.709	1.00	19.19	A
ATOM	209	CB	ARG	A	25	22.552	3.343	15.287	1.00	20.85	A
ATOM	210	CG	ARG	A	25	22.674	1.959	14.627	1.00	23.87	A
ATOM	211	CD	ARG	A</							

Figure 7F

004574 22400

ATOM	328	CB	LYS	A	27	16.330	6.994	16.805	1.00	19.01	A
ATOM	229	CG	LYS	A	27	16.266	8.210	15.876	1.00	22.27	A
ATOM	230	CD	LYS	A	27	15.275	7.984	14.711	1.00	24.03	A
ATOM	231	CE	LYS	A	27	13.860	7.664	15.161	1.00	24.41	A
ATOM	232	NZ	LYS	A	27	13.173	8.848	15.714	1.00	27.04	A
ATOM	233	C	LYS	A	27	17.326	6.097	18.969	1.00	18.17	A
ATOM	234	O	LYS	A	27	16.767	6.388	20.013	1.00	18.33	A
ATOM	235	N	LYS	A	28	17.871	4.896	18.775	1.00	17.00	A
ATOM	236	CA	LYS	A	28	17.788	3.867	19.790	1.00	17.21	A
ATOM	237	CB	LYS	A	28	18.244	2.503	19.223	1.00	18.92	A
ATOM	238	CG	LYS	A	28	17.288	1.982	18.164	1.00	24.56	A
ATOM	239	CD	LYS	A	28	17.833	0.732	17.464	1.00	26.88	A
ATOM	240	CE	LYS	A	28	16.950	0.371	16.260	1.00	28.84	A
ATOM	241	NZ	LYS	A	28	17.284	-0.938	15.592	1.00	31.36	A
ATOM	242	C	LYS	A	28	18.618	4.257	21.016	1.00	17.36	A
ATOM	243	O	LYS	A	28	18.169	4.066	22.165	1.00	17.54	A
ATOM	244	N	LEU	A	29	19.794	4.835	20.793	1.00	16.84	A
ATOM	245	CA	LEU	A	29	20.642	5.234	21.912	1.00	16.41	A
ATOM	246	CB	LEU	A	29	22.077	5.529	21.453	1.00	16.26	A
ATOM	247	CG	LEU	A	29	23.050	6.048	22.515	1.00	16.76	A
ATOM	248	CD1	LEU	A	29	23.062	5.096	23.701	1.00	16.47	A
ATOM	249	CD2	LEU	A	29	24.450	6.201	21.885	1.00	17.67	A
ATOM	250	C	LEU	A	29	20.023	6.429	22.606	1.00	16.92	A
ATOM	251	O	LEU	A	29	20.027	6.503	23.859	1.00	16.36	A
ATOM	252	N	LEU	A	30	19.447	7.343	21.820	1.00	15.57	A
ATOM	253	CA	LEU	A	30	18.818	8.519	22.424	1.00	15.77	A
ATOM	254	CB	LEU	A	30	18.401	9.501	21.298	1.00	15.65	A
ATOM	255	CG	LEU	A	30	17.717	10.780	21.696	1.00	17.55	A
ATOM	256	CD1	LEU	A	30	18.557	11.504	22.722	1.00	16.71	A
ATOM	257	CD2	LEU	A	30	17.552	11.602	20.399	1.00	18.10	A
ATOM	258	C	LEU	A	30	17.659	8.067	23.288	1.00	16.42	A
ATOM	259	O	LEU	A	30	17.466	8.604	24.399	1.00	17.55	A
ATOM	260	N	GLN	A	31	16.903	7.053	22.862	1.00	16.79	A
ATOM	261	CA	GLN	A	31	15.816	6.564	23.692	1.00	18.13	A
ATOM	262	CB	GLN	A	31	14.945	5.593	22.886	1.00	21.45	A
ATOM	263	CG	GLN	A	31	14.119	6.358	21.834	1.00	24.92	A
ATOM	264	CD	GLN	A	31	13.196	7.437	22.424	1.00	26.81	A
ATOM	265	OE1	GLN	A	31	12.913	8.459	21.786	1.00	28.75	A
ATOM	266	NE2	GLN	A	31	12.713	7.207	23.648	1.00	29.86	A
ATOM	267	C	GLN	A	31	16.319	5.958	25.008	1.00	17.24	A
ATOM	268	O	GLN	A	31	15.655	6.092	26.038	1.00	17.79	A
ATOM	269	N	LEU	A	32	17.494	5.307	24.987	1.00	15.77	A
ATOM	270	CA	LEU	A	32	18.070	4.755	26.209	1.00	14.63	A
ATOM	271	CB	LEU	A	32	19.314	3.932	25.911	1.00	16.13	A
ATOM	272	CG	LEU	A	32	19.015	2.574	25.275	1.00	18.58	A
ATOM	273	CD1	LEU	A	32	20.291	1.961	24.770	1.00	20.70	A
ATOM	274	CD2	LEU	A	32	18.337	1.698	26.315	1.00	22.17	A
ATOM	275	C	LEU	A	32	18.449	5.895	27.140	1.00	13.68	A
ATOM	276	O	LEU	A	32	18.258	5.774	28.357	1.00	13.31	A
ATOM	277	N	THR	A	33	18.980	6.991	26.600	1.00	13.42	A
ATOM	278	CA	THR	A	33	19.348	8.081	27.500	1.00	12.96	A
ATOM	279	CB	THR	A	33	20.236	9.134	26.820	1.00	13.48	A
ATOM	280	OG1	THR	A	33	19.530	9.745	25.733	1.00	15.60	A
ATOM	281	CG2	THR	A	33	21.567	8.508	26.358	1.00	15.01	A
ATOM	282	C	THR	A	33	18.124	8.742	28.117	1.00	13.65	A
ATOM	283	O	THR	A	33	18.159	9.169	29.285	1.00	12.67	A
ATOM	284	N	VAL	A	34	17.038	8.838	27.345	1.00	13.20	A
ATOM	285	CA	VAL	A	34	15.804	9.410	27.863	1.00	13.38	A

Figure 7G

ATOM	286	CB	VAL	A	34	14.708	9.498	26.773	1.00	14.31	A
ATOM	287	CG1	VAL	A	34	13.380	9.811	27.382	1.00	15.35	A
ATOM	288	CG2	VAL	A	34	15.096	10.517	25.710	1.00	15.04	A
ATOM	289	C	VAL	A	34	15.326	8.526	29.041	1.00	12.55	A
ATOM	290	O	VAL	A	34	14.997	9.016	30.131	1.00	13.43	A
ATOM	291	N	TRP	A	35	15.354	7.210	28.857	1.00	13.04	A
ATOM	292	CA	TRP	A	35	14.946	6.289	29.908	1.00	13.11	A
ATOM	293	CB	TRP	A	35	14.988	4.861	29.319	1.00	14.19	A
ATOM	294	CG	TRP	A	35	14.672	3.785	30.334	1.00	13.43	A
ATOM	295	CD2	TRP	A	35	15.610	3.101	31.191	1.00	13.26	A
ATOM	296	CE2	TRP	A	35	14.860	2.165	31.963	1.00	15.57	A
ATOM	297	CE3	TRP	A	35	16.990	3.196	31.393	1.00	15.49	A
ATOM	298	CD1	TRP	A	35	13.454	3.258	30.609	1.00	17.15	A
ATOM	299	NE1	TRP	A	35	13.553	2.281	31.572	1.00	17.80	A
ATOM	300	CZ2	TRP	A	35	15.459	1.324	32.905	1.00	15.31	A
ATOM	301	CZ3	TRP	A	35	17.600	2.355	32.349	1.00	16.17	A
ATOM	302	CH2	TRP	A	35	16.815	1.437	33.090	1.00	14.74	A
ATOM	303	C	TRP	A	35	15.869	6.429	31.141	1.00	13.13	A
ATOM	304	O	TRP	A	35	15.418	6.409	32.278	1.00	12.76	A
ATOM	305	N	GLY	A	36	17.176	6.556	30.893	1.00	12.50	A
ATOM	306	CA	GLY	A	36	18.118	6.668	31.998	1.00	12.50	A
ATOM	307	C	GLY	A	36	17.887	7.936	32.817	1.00	11.58	A
ATOM	308	O	GLY	A	36	17.917	7.875	34.042	1.00	11.70	A
ATOM	309	N	ILE	A	37	17.656	9.084	32.174	1.00	11.85	A
ATOM	310	CA	ILE	A	37	17.383	10.303	32.884	1.00	11.18	A
ATOM	311	CB	ILE	A	37	17.262	11.439	31.882	1.00	11.22	A
ATOM	312	CG2	ILE	A	37	16.680	12.660	32.600	1.00	13.25	A
ATOM	313	CG1	ILE	A	37	18.636	11.739	31.281	1.00	12.70	A
ATOM	314	CD1	ILE	A	37	18.571	12.560	29.955	1.00	13.00	A
ATOM	315	C	ILE	A	37	16.082	10.105	33.703	1.00	11.99	A
ATOM	316	O	ILE	A	37	16.026	10.526	34.860	1.00	12.24	A
ATOM	317	N	LYS	A	38	15.069	9.465	33.094	1.00	11.84	A
ATOM	318	CA	LYS	A	38	13.825	9.215	33.809	1.00	13.62	A
ATOM	319	CB	LYS	A	38	12.840	8.512	32.861	1.00	15.00	A
ATOM	320	CG	LYS	A	38	11.429	8.437	33.369	1.00	17.76	A
ATOM	321	CD	LYS	A	38	10.545	7.835	32.247	1.00	20.78	A
ATOM	322	CE	LYS	A	38	9.046	7.955	32.600	1.00	25.34	A
ATOM	323	NZ	LYS	A	38	8.721	7.069	33.722	1.00	29.03	A
ATOM	324	C	LYS	A	38	14.060	8.399	35.083	1.00	12.64	A
ATOM	325	O	LYS	A	38	13.490	8.724	36.163	1.00	12.58	A
ATOM	326	N	GLN	A	39	14.916	7.371	35.001	1.00	11.99	A

Figure 7H

Figure 71

001227-000000

ATOM	402	SG	DCS	D	3	19.502	-2.991	25.840	1.00	30.98	E
ATOM	403	N	DLU	D	4	15.813	-4.736	28.474	1.00	31.68	B
ATOM	404	CA	DLU	D	4	14.782	-5.702	28.834	1.00	32.07	B
ATOM	405	CB	DLU	D	4	13.397	-5.090	28.574	1.00	33.43	B
ATOM	406	CG	DLU	D	4	13.060	-4.844	27.093	1.00	35.53	B
ATOM	407	CD	DLU	D	4	13.663	-3.568	26.500	1.00	36.29	B
ATOM	408	OE1	DLU	D	4	14.422	-2.859	27.182	1.00	37.11	B
ATOM	409	OE2	DLU	D	4	13.367	-3.264	25.323	1.00	37.45	B
ATOM	410	C	DLU	D	4	14.875	-6.180	30.276	1.00	31.86	B
ATOM	411	O	DLU	D	4	14.832	-7.381	30.553	1.00	32.10	B
ATOM	412	N	DLA	D	5	15.022	-5.237	31.196	1.00	30.98	B
ATOM	413	CA	DLA	D	5	15.098	-5.566	32.611	1.00	30.61	B
ATOM	414	CB	DLA	D	5	14.984	-4.296	33.406	1.00	30.83	B
ATOM	415	C	DLA	D	5	16.362	-6.340	33.008	1.00	30.19	B
ATOM	416	O	DLA	D	5	16.387	-7.044	34.027	1.00	30.60	B
ATOM	417	N	DRG	D	6	17.418	-6.202	32.216	1.00	29.09	B
ATOM	418	CA	DRG	D	6	18.673	-6.893	32.489	1.00	28.71	B
ATOM	419	CB	DRG	D	6	18.480	-8.408	32.369	1.00	31.46	B
ATOM	420	CG	DRG	D	6	18.169	-8.847	30.969	1.00	34.88	B
ATOM	421	CD	DRG	D	6	19.397	-8.762	30.070	1.00	37.42	B
ATOM	422	NE	DRG	D	6	19.715	-7.408	29.607	1.00	40.28	B
ATOM	423	CZ	DRG	D	6	20.121	-7.134	28.370	1.00	40.89	B
ATOM	424	NH1	DRG	D	6	20.248	-8.118	27.481	1.00	42.76	B
ATOM	425	NH2	DRG	D	6	20.409	-5.891	28.015	1.00	42.55	B
ATOM	426	C	DRG	D	6	19.313	-6.582	33.833	1.00	27.29	B
ATOM	427	O	DRG	D	6	19.994	-7.423	34.421	1.00	27.43	B
ATOM	428	N	DIS	D	7	19.100	-5.379	34.342	1.00	24.49	B
ATOM	429	CA	DIS	D	7	19.731	-5.018	35.624	1.00	22.04	B
ATOM	430	CB	DIS	D	7	18.970	-3.888	36.284	1.00	22.68	B
ATOM	431	CG	DIS	D	7	17.655	-4.321	36.854	1.00	22.88	B
ATOM	432	CD2	DIS	D	7	17.178	-5.567	37.104	1.00	24.08	B
ATOM	433	ND1	DIS	D	7	16.650	-3.445	37.187	1.00	25.78	B
ATOM	434	CE1	DIS	D	7	15.595	-4.134	37.608	1.00	26.45	B
ATOM	435	NE2	DIS	D	7	15.894	-5.419	37.562	1.00	25.11	B
ATOM	436	C	DIS	D	7	21.156	-4.636	35.329	1.00	21.84	B
ATOM	437	O	DIS	D	7	21.412	-3.743	34.536	1.00	20.32	B
ATOM	438	N	DRG	D	8	22.091	-5.298	36.003	1.00	20.33	B
ATOM	439	CA	DRG	D	8	23.494	-5.122	35.778	1.00	19.80	B
ATOM	440	CB	DRG	D	8	24.284	-5.994	36.755	1.00	20.87	B
ATOM	441	CG	DRG	D	8	24.175	-7.428	36.459	1.00	26.97	B
ATOM	442	CD	DRG	D	8	24.743	-8.207	37.631	1.00	29.07	B
ATOM	443	NE	DRG	D	8	24.581	-9.603	37.325	1.00	31.54	B
ATOM	444	CZ	DRG	D	8	25.258	-10.189	36.352	1.00	31.94	B
ATOM	445	NH1	DRG	D	8	26.139	-9.485	35.658	1.00	33.88	B
ATOM	446	NH2	DRG	D	8	24.987	-11.432	36.027	1.00	33.88	B
ATOM	447	C	DRG	D	8	23.985	-3.711	35.873	1.00	17.95	B
ATOM	448	O	DRG	D	8	24.856	-3.361	35.124	1.00	17.42	B
ATOM	449	N	DLU	D	9	23.407	-2.934	36.783	1.00	16.93	B
ATOM	450	CA	DLU	D	9	23.900	-1.578	36.951	1.00	15.49	B
ATOM	451	CB	DLU	D	9	23.358	-0.954	38.261	1.00	16.03	B
ATOM	452	CG	DLU	D	9	21.876	-0.652	38.323	1.00	16.75	B
ATOM	453	CD	DLU	D	9	20.996	-1.816	38.786	1.00	16.82	B
ATOM	454	OE1	DLU	D	9	21.407	-2.982	38.584	1.00	19.63	B
ATOM	455	OE2	DLU	D	9	19.933	-1.498	39.310	1.00	20.12	B
ATOM	456	C	DLU	D	9	23.601	-0.717	35.747	1.00	15.97	B
ATOM	457	O	DLU	D	9	24.142	0.383	35.655	1.00	15.24	B
ATOM	458	N	DRP	D	10	22.747	-1.186	34.844	1.00	15.66	B
ATOM	459	CA	DRP	D	10	22.462	-0.435	35.611	1.00	15.31	B

Figure 7J

ATOM	460	CE	DRP	D	10	20.960	-0.187	33.430	1.00	16.05	B
ATOM	461	CG	DRP	D	10	20.354	0.791	34.410	1.00	15.28	B
ATOM	462	CD2	DRP	D	10	20.504	2.200	34.384	1.00	15.28	B
ATOM	463	CE2	DRP	D	10	19.734	2.730	35.424	1.00	15.74	B
ATOM	464	CE3	DRP	D	10	21.237	3.075	33.563	1.00	15.47	B
ATOM	465	CD1	DRP	D	10	19.504	0.512	35.449	1.00	16.40	B
ATOM	466	NE1	DRP	D	10	19.122	1.676	36.073	1.00	17.22	B
ATOM	467	CZ2	DRP	D	10	19.650	4.107	35.666	1.00	15.81	B
ATOM	468	CZ3	DRP	D	10	21.174	4.444	33.805	1.00	14.93	B
ATOM	469	CH2	DRP	D	10	20.382	4.935	34.850	1.00	15.26	B
ATOM	470	C	DRP	D	10	23.000	-1.140	32.376	1.00	17.32	B
ATOM	471	O	DRP	D	10	22.790	-0.682	31.244	1.00	16.59	B
ATOM	472	N	DLA	D	11	23.744	-2.227	32.572	1.00	17.72	B
ATOM	473	CA	DLA	D	11	24.253	-2.940	31.407	1.00	18.88	B
ATOM	474	CB	DLA	D	11	25.034	-4.168	31.867	1.00	20.11	B
ATOM	475	C	DLA	D	11	25.126	-2.074	30.501	1.00	18.95	B
ATOM	476	O	DLA	D	11	25.078	-2.221	29.267	1.00	21.13	B
ATOM	477	N	DRP	D	12	25.884	-1.142	31.084	1.00	17.86	B
ATOM	478	CA	DRP	D	12	26.759	-0.275	30.317	1.00	17.72	B
ATOM	479	CB	DRP	D	12	27.586	0.645	31.239	1.00	18.43	B
ATOM	480	CG	DRP	D	12	26.725	1.588	32.059	1.00	16.68	B
ATOM	481	CD2	DRP	D	12	26.285	2.900	31.676	1.00	16.49	B
ATOM	482	CE2	DRP	D	12	25.459	3.371	32.706	1.00	15.68	B
ATOM	483	CE3	DRP	D	12	26.519	3.714	30.561	1.00	17.14	B
ATOM	484	CD1	DRP	D	12	26.177	1.335	33.256	1.00	15.60	B
ATOM	485	NE1	DRP	D	12	25.402	2.400	33.668	1.00	15.74	B
ATOM	486	CZ2	DRP	D	12	24.842	4.628	32.664	1.00	15.78	B
ATOM	487	CZ3	DRP	D	12	25.904	4.977	30.525	1.00	17.42	B
ATOM	488	CH2	DRP	D	12	25.090	5.406	31.550	1.00	16.81	B
ATOM	489	C	DRP	D	12	25.913	0.577	29.346	1.00	18.81	B
ATOM	490	O	DRP	D	12	26.347	0.870	28.231	1.00	20.05	B
ATOM	491	N	DEU	D	13	24.740	1.020	29.790	1.00	17.43	B
ATOM	492	CA	DEU	D	13	23.915	1.866	28.926	1.00	17.59	B
ATOM	493	CB	DEU	D	13	22.883	2.647	29.756	1.00	15.97	B
ATOM	494	CG	DEU	D	13	21.857	3.489	28.971	1.00	15.31	B
ATOM	495	CD1	DEU	D	13	22.559	4.585	28.204	1.00	16.99	B
ATOM	496	CD2	DEU	D	13	20.886	4.105	29.938	1.00	16.07	B
ATOM	497	C	DEU	D	13	23.265	1.011	27.847	1.00	19.32	B
ATOM	498	O	DEU	D	13	23.224	1.429	26.702	1.00	20.12	B
ATOM	499	N	DCS	D	14	22.775	-0.280	28.199	1.00	20.93	B
ATOM	500	CA	DCS	D	14	22.190	-1.046	27.196	1.00		

Figure 7K

not shown

ATOM	518	OH2	WAT	W	2	30.822	2.444	-19.357	1.00	52.17	W
ATOM	519	OH2	WAT	W	3	30.369	13.971	-17.693	1.00	37.23	W
ATOM	520	OH2	WAT	W	4	27.699	12.875	-16.588	1.00	46.63	W
ATOM	521	OH2	WAT	W	5	23.417	1.727	-13.168	1.00	48.41	W
ATOM	522	OH2	WAT	W	6	24.012	1.401	-16.007	1.00	58.65	W
ATOM	523	OH2	WAT	W	7	16.572	3.069	-7.418	1.00	36.12	W
ATOM	524	OH2	WAT	W	8	32.381	11.028	-8.334	1.00	55.01	W
ATOM	525	OH2	WAT	W	9	33.753	7.275	-10.261	1.00	53.14	W
ATOM	526	OH2	WAT	W	10	20.318	-0.862	-12.067	1.00	28.89	W
ATOM	527	OH2	WAT	W	11	26.434	1.459	-10.129	1.00	42.04	W
ATOM	528	OH2	WAT	W	12	27.878	0.323	-12.146	1.00	55.95	W
ATOM	529	OH2	WAT	W	13	31.427	0.259	-10.741	1.00	52.47	W
ATOM	530	OH2	WAT	W	14	29.889	8.411	-6.889	1.00	56.49	W
ATOM	531	OH2	WAT	W	15	22.532	1.843	-4.021	1.00	32.19	W
ATOM	532	OH2	WAT	W	16	23.814	-0.534	-4.336	1.00	39.56	W
ATOM	533	OH2	WAT	W	17	19.996	1.598	-5.292	1.00	33.28	W
ATOM	534	OH2	WAT	W	18	25.262	-3.040	-8.386	1.00	28.37	W
ATOM	535	OH2	WAT	W	19	22.556	0.000	0.001	1.00	30.95	W
ATOM	536	OH2	WAT	W	20	24.369	-1.421	-1.823	1.00	29.32	W
ATOM	537	OH2	WAT	W	21	29.134	-0.583	-6.291	1.00	46.18	W
ATOM	538	OH2	WAT	W	22	27.394	2.286	-5.533	1.00	43.67	W
ATOM	539	OH2	WAT	W	23	26.774	0.049	-4.387	1.00	45.47	W
ATOM	540	OH2	WAT	W	24	30.008	5.236	1.507	1.00	52.80	W
ATOM	541	OH2	WAT	W	25	27.776	4.560	0.356	1.00	42.94	W
ATOM	542	OH2	WAT	W	26	32.018	6.237	0.261	1.00	53.15	W
ATOM	543	OH2	WAT	W	28	18.650	4.426	-0.423	1.00	34.71	W
ATOM	544	OH2	WAT	W	29	18.919	1.842	-1.284	1.00	42.23	W
ATOM	545	OH2	WAT	W	30	11.826	6.239	7.700	1.00	59.49	W
ATOM	546	OH2	WAT	W	31	13.683	5.469	2.919	1.00	52.76	W
ATOM	547	OH2	WAT	W	32	16.956	4.594	1.380	1.00	47.84	W
ATOM	548	OH2	WAT	W	33	17.260	2.099	7.679	1.00	46.32	W
ATOM	549	OH2	WAT	W	34	17.636	1.737	-4.073	1.00	51.94	W
ATOM	550	OH2	WAT	W	35	16.221	5.835	9.764	1.00	30.19	W
ATOM	551	OH2	WAT	W	36	26.030	8.926	8.979	1.00	51.32	W
ATOM	552	OH2	WAT	W	37	13.758	2.898	9.624	1.00	52.05	W
ATOM	553	OH2	WAT	W	38	14.899	5.914	11.925	1.00	35.86	W
ATOM	554	OH2	WAT	W	39	19.841	0.030	14.724	1.00	45.90	W
ATOM	555	OH2	WAT	W	40	13.772	2.335	12.179	1.00	50.60	W
ATOM	556	OH2	WAT	W	41	13.367	0.805	6.229	1.00	51.80	W
ATOM	557	OH2	WAT	W	42	15.587	3.501	15.845	1.00	30.05	W
ATOM	558	OH2	WAT	W	43	14.280	4.098	13.819	1.00	48.74	W
ATOM	559	OH2	WAT	W	44	14.273	3.983	18.042	1.00	32.62	W
ATOM	560	OH2	WAT	W	45	14.275	2.720	20.720	1.00	40.19	W
ATOM	561	OH2	WAT	W	46	21.969	2.228	18.885	1.00	22.32	W
ATOM	562	OH2	WAT	W	47	21.588	1.778	21.594	1.00	28.43	W
ATOM	563	OH2	WAT	W	48	11.908	3.300	22.023	1.00	50.50	W
ATOM	564	OH2	WAT	W	49	13.679	0.626	18.643	1.00	46.64	W
ATOM	565	OH2	WAT	W	50	16.369	2.196	22.597	1.00	30.08	W
ATOM	566	OH2	WAT	W	51	12.828	6.527	18.634	1.00	37.29	W
ATOM	567	OH2	WAT	W	52	24.603	2.631	19.581	1.00	25.55	W
ATOM	568	OH2	WAT	W	53	11.867	0.791	23.131	1.00	58.27	W
ATOM	569	OH2	WAT	W	54	24.646	5.366	17.812	1.00	50.24	W
ATOM	570	OH2	WAT	W	55	20.954	0.091	17.131	1.00	49.14	W
ATOM	571	OH2	WAT	W	56	19.747	-0.562	21.394	1.00	36.92	W
ATOM	572	OH2	WAT	W	57	14.819	8.442	19.922	1.00	33.61	W
ATOM	573	OH2	WAT	W	58	10.854	5.349	19.724	1.00	45.89	W
ATOM	574	OH2	WAT	W	59	10.710	9.378	19.376	1.00	37.52	W
ATOM	575	OH2	WAT	W	60	10.497	10.303	21.845	1.00	34.96	W

Figure 7L

ATOM	576	OH2	WAT	W	61	12.866	5.691	26.354	1.00	29.86	W
ATOM	577	OH2	WAT	W	62	10.758	7.878	25.495	1.00	42.32	W
ATOM	578	OH2	WAT	W	63	11.782	6.555	28.773	1.00	29.65	W
ATOM	579	OH2	WAT	W	64	10.296	8.472	27.988	1.00	37.31	W
ATOM	580	OH2	WAT	W	65	13.315	2.342	26.849	1.00	43.22	W
ATOM	581	OH2	WAT	W	66	29.863	-1.693	28.654	1.00	38.41	W
ATOM	582	OH2	WAT	W	67	16.468	-1.186	26.444	1.00	32.71	W
ATOM	583	OH2	WAT	W	68	20.934	12.065	25.212	1.00	18.68	W
ATOM	584	OH2	WAT	W	69	7.101	5.989	26.485	1.00	48.02	W
ATOM	585	OH2	WAT	W	70	7.226	10.744	27.574	1.00	33.30	W
ATOM	586	OH2	WAT	W	71	16.382	-1.374	34.997	1.00	34.36	W
ATOM	587	OH2	WAT	W	72	17.474	-0.717	38.167	1.00	28.82	W
ATOM	588	OH2	WAT	W	73	17.984	-2.951	33.186	1.00	27.39	W
ATOM	589	OH2	WAT	W	74	16.999	1.929	37.830	1.00	37.09	W
ATOM	590	OH2	WAT	W	75	20.595	3.071	39.121	1.00	19.51	W
ATOM	591	OH2	WAT	W	76	14.326	5.004	39.584	1.00	20.31	W
ATOM	592	OH2	WAT	W	77	11.973	4.544	38.034	1.00	32.93	W
ATOM	593	OH2	WAT	W	78	18.317	4.417	39.397	1.00	44.00	W
ATOM	594	OH2	WAT	W	79	10.983	-2.804	30.948	1.00	52.39	W
ATOM	595	OH2	WAT	W	80	11.064	0.945	32.640	1.00	30.78	W
ATOM	596	OH2	WAT	W	81	12.861	0.902	39.566	1.00	51.74	W
ATOM	597	OH2	WAT	W	82	14.353	-1.379	39.210	1.00	48.06	W
ATOM	598	OH2	WAT	W	83	13.014	-3.417	36.263	1.00	46.54	W
ATOM	599	OH2	WAT	W	84	11.101	-2.319	39.669	1.00	61.24	W
ATOM	600	OH2	WAT	W	85	20.879	-3.825	31.838	1.00	26.25	W
ATOM	601	OH2	WAT	W	86	24.470	-4.753	28.192	1.00	36.86	W
ATOM	602	OH2	WAT	W	87	22.117	-5.700	29.831	1.00	38.03	W
ATOM	603	OH2	WAT	W	88	19.685	0.721	41.041	1.00	28.21	W
ATOM	604	OH2	WAT	W	89	20.274	5.127	40.337	1.00	32.29	W
ATOM	605	OH2	WAT	W	90	10.072	4.538	29.943	1.00	33.10	W
ATOM	606	OH2	WAT	W	91	10.573	4.216	33.496	1.00	33.22	W
ATOM	607	OH2	WAT	W	92	10.336	5.922	36.364	1.00	48.48	W
ATOM	608	OH2	WAT	W	93	9.113	5.209	40.332	1.00	51.71	W
ATOM	609	OH2	WAT	W	94	9.980	8.713	42.573	1.00	24.98	W
ATOM	610	OH2	WAT	W	95	17.708	6.542	-1.798	1.00	36.93	W
ATOM	611	OH2	WAT	W	96	10.278	11.397	38.730	1.00	17.13	W
ATOM	612	OH2	WAT	W	97	11.290	10.478	36.184	1.00	15.62	W
ATOM	613	OH2	WAT	W	98	8.444	12.988	37.395	1.00	17.25	W
ATOM	614	OH2	WAT	W	99	8.735	9.911	40.361	1.00	25.18	W
ATOM	615	OH2	WAT	W	100	6.665	11.917	35.86			

Figure 7M

ATOM	634	OH2	WAT	W	119	33.766	4.315	-14.106	1.00	57.44	W
ATOM	635	OH2	WAT	W	120	26.831	7.497	7.075	1.00	40.38	W
ATOM	636	OH2	WAT	W	121	26.562	8.206	4.240	1.00	32.00	W
ATOM	637	OH2	WAT	W	122	29.081	7.039	3.251	1.00	46.30	W
ATOM	638	OH2	WAT	W	123	22.080	-0.975	10.516	1.00	39.31	W
ATOM	639	OH2	WAT	W	124	28.185	3.991	13.044	1.00	45.28	W
ATOM	640	OH2	WAT	W	125	29.400	7.324	10.996	1.00	52.21	W
ATOM	641	OH2	WAT	W	126	12.966	3.595	24.673	1.00	59.42	W
ATOM	642	OH2	WAT	W	127	8.932	7.961	36.476	1.00	45.85	W
ATOM	643	OH2	WAT	W	128	12.712	5.206	41.719	1.00	38.55	W
ATOM	644	OH2	WAT	W	129	9.431	10.564	47.230	1.00	35.27	W
ATOM	645	OH2	WAT	W	130	6.643	9.576	45.596	1.00	44.00	W
ATOM	646	OH2	WAT	W	131	21.501	13.657	45.856	1.00	43.49	W
ATOM	647	OH2	WAT	W	132	19.368	14.112	46.567	1.00	41.15	W
ATOM	648	OH2	WAT	W	133	20.913	12.058	48.230	1.00	36.86	W
ATOM	649	OH2	WAT	W	134	13.556	4.967	44.137	1.00	49.55	W
ATOM	650	OH2	WAT	W	135	17.568	0.000	0.010	1.00	54.94	W
ATOM	651	OH2	WAT	W	136	17.847	-0.139	11.093	1.00	42.03	W
ATOM	652	OH2	WAT	W	137	25.734	4.074	15.641	1.00	35.36	W
ATOM	653	OH2	WAT	W	138	8.107	7.930	38.831	1.00	37.47	W
ATOM	654	OH2	WAT	W	139	10.614	4.603	44.378	1.00	61.10	W
ATOM	655	OH2	WAT	W	140	14.180	-9.552	32.610	1.00	37.66	W
ATOM	656	OH2	WAT	W	141	26.549	-4.072	22.858	1.00	48.05	W
ATOM	657	OH2	WAT	W	142	21.688	-2.141	22.847	1.00	36.75	W
ATOM	658	OH2	WAT	W	143	15.457	1.462	27.799	1.00	38.11	W
ATOM	659	OH2	WAT	W	144	18.956	16.356	45.521	1.00	36.93	W
ATOM	660	OH2	WAT	W	145	15.655	2.938	40.183	1.00	40.77	W
ATOM	661	OH2	WAT	W	146	15.688	-1.613	19.777	1.00	47.04	W
ATOM	662	OH2	WAT	W	147	26.880	-5.627	28.327	1.00	44.89	W
ATOM	663	OH2	WAT	W	148	28.682	-5.605	33.707	1.00	43.34	W
ATOM	664	OH2	WAT	W	149	28.220	11.179	-23.836	1.00	53.67	W
ATOM	665	OH2	WAT	W	150	27.905	3.222	-7.774	1.00	44.54	W
ATOM	666	OH2	WAT	W	151	15.403	-11.541	32.995	1.00	47.59	W
TER											
END											

Figure 7N

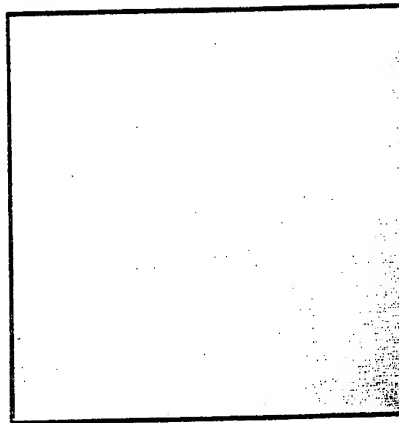
Inhibition of HIV-1 Membrane Fusion by a D-Peptide

Figure 8A



Syncytia Assay with no D-peptide

Figure 8B



Syncytia Assay with [100 μM] peptide

007221 21251260

Figure 9A

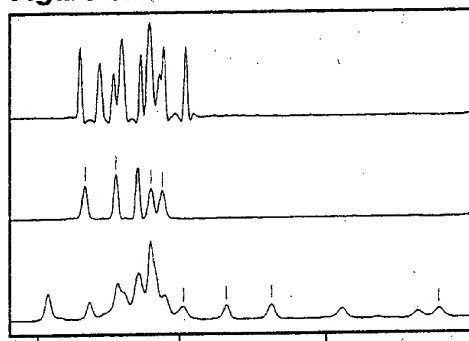


Figure 9C

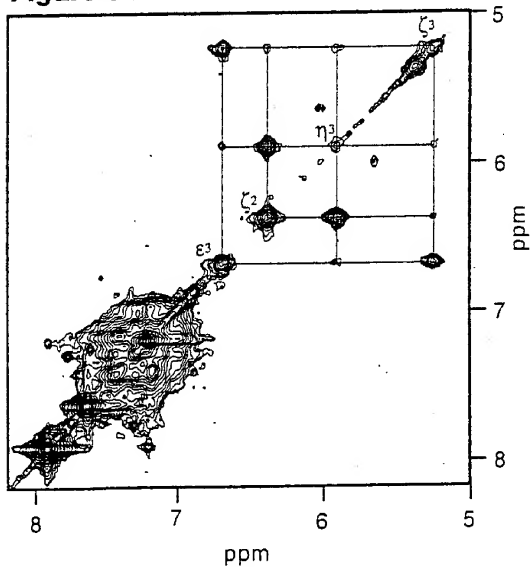


Figure 9B

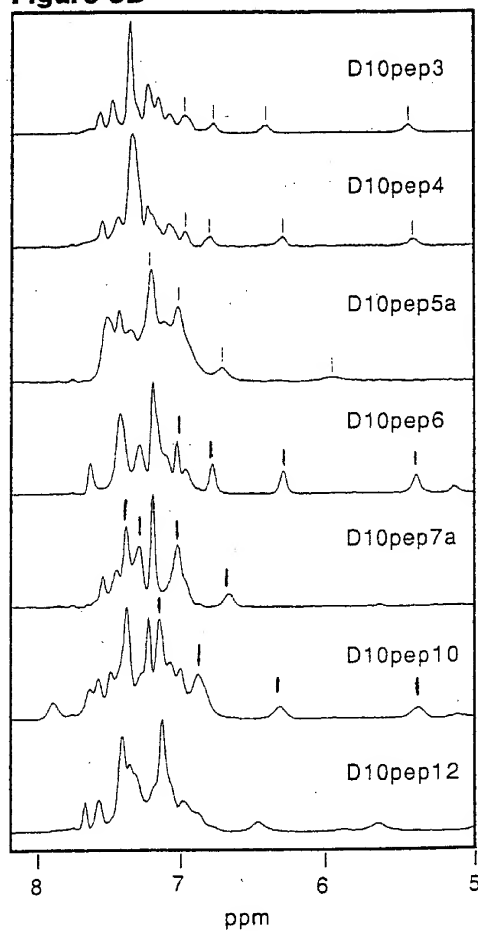
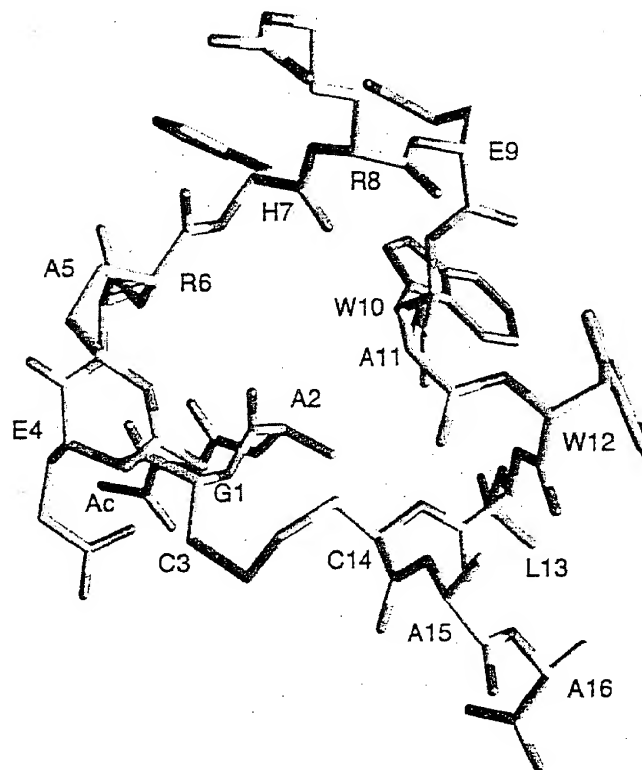


Figure 10: Conformation of D10pep1 in complex with IQN17



00745742-122100

Figure 11.A

ATOM	52	CG	GLU	A	6	17.636	20.359	33.480	1.00	56.46	A
ATOM	53	CD	GLU	A	6	17.293	19.009	34.119	1.00	56.33	A
ATOM	54	OE1	GLU	A	6	17.702	18.790	35.278	1.00	53.43	A
ATOM	55	OE2	GLU	A	6	16.644	18.157	33.458	1.00	55.03	A
ATOM	56	C	GLU	A	6	17.873	23.977	34.926	1.00	54.87	A
ATOM	57	O	GLU	A	6	16.793	24.509	35.137	1.00	52.82	A
ATOM	58	N	ASP	A	7	18.986	24.300	35.572	1.00	55.62	A
ATOM	59	CA	ASP	A	7	19.039	25.336	36.597	1.00	56.65	A
ATOM	60	CB	ASP	A	7	20.291	25.162	37.451	1.00	57.46	A
ATOM	61	CG	ASP	A	7	20.010	24.471	38.762	1.00	57.37	A
ATOM	62	OD1	ASP	A	7	19.180	23.534	38.775	1.00	53.78	A
ATOM	63	OD2	ASP	A	7	20.637	24.862	39.771	1.00	57.66	A
ATOM	64	C	ASP	A	7	19.034	26.745	36.041	1.00	56.99	A
ATOM	65	O	ASP	A	7	18.516	27.662	36.678	1.00	55.43	A
ATOM	66	N	LYS	A	8	19.632	26.945	34.873	1.00	58.30	A
ATOM	67	CA	LYS	A	8	19.642	28.290	34.312	1.00	59.87	A
ATOM	68	CB	LYS	A	8	20.971	28.599	33.612	1.00	62.61	A
ATOM	69	CG	LYS	A	8	22.203	28.372	34.487	1.00	66.85	A
ATOM	70	CD	LYS	A	8	23.232	29.498	34.357	1.00	70.21	A
ATOM	71	CE	LYS	A	8	22.915	30.676	35.293	1.00	72.00	A
ATOM	72	NZ	LYS	A	8	21.583	31.323	35.091	1.00	72.05	A
ATOM	73	C	LYS	A	8	18.467	28.481	33.354	1.00	58.08	A
ATOM	74	O	LYS	A	8	18.145	29.609	32.969	1.00	56.44	A
ATOM	75	N	ILE	A	9	17.835	27.376	32.967	1.00	55.29	A
ATOM	76	CA	ILE	A	9	16.668	27.436	32.099	1.00	56.69	A
ATOM	77	CB	ILE	A	9	16.325	26.052	31.486	1.00	54.89	A
ATOM	78	CG2	ILE	A	9	14.892	26.067	30.915	1.00	54.20	A
ATOM	79	CG1	ILE	A	9	17.373	25.676	30.423	1.00	55.96	A
ATOM	80	CD1	ILE	A	9	17.131	24.339	29.717	1.00	54.22	A
ATOM	81	C	ILE	A	9	15.526	27.876	33.018	1.00	57.98	A
ATOM	82	O	ILE	A	9	14.603	28.572	32.616	1.00	55.85	A
ATOM	83	N	GLU	A	10	15.626	27.458	34.271	1.00	59.96	A
ATOM	84	CA	GLU	A	10	14.641	27.788	35.283	1.00	61.12	A
ATOM	85	CB	GLU	A	10	14.850	26.901	36.510	1.00	63.01	A
ATOM	86	CG	GLU	A	10	13.846	27.117	37.618	1.00	66.89	A
ATOM	87	CD	GLU	A	10	14.387	26.672	38.955	1.00	68.37	A
ATOM	88	OE1	GLU	A	10	14.844	25.510	39.054	1.00	67.70	A
ATOM	89	OE2	GLU	A	10	14.355	27.487	39.903	1.00	68.42	A
ATOM	90	C	GLU	A	10	14.872	29.243	35.664	1.00	59.41	A
ATOM	91	O	GLU	A	10	13.947	29.958	36.037	1.00	59.95	A
ATOM	92	N	GLU	A	11	16.127	29.663	35.565	1.00	57.16	A
ATOM	93	CA	GLU	A	11	16.524	31.024	35.893	1.00	55.88	A
ATOM	94	CB	GLU	A	11	18.042	31.095	36.019	1.00	58.17	A
ATOM	95	CG	GLU	A	11	18.569	32.375	36.627	1.00	62.73	A
ATOM	96	CD	GLU	A	11	18.459	32.382	38.139	1.00	67.75	A
ATOM	97	OE1	GLU	A	11	19.101	31.512	38.782	1.00	67.91	A
ATOM	98	OE2	GLU	A	11	17.736	33.249	38.681	1.00	68.84	A
ATOM	99	C	GLU	A	11	16.056	31.976	34.789	1.00	54.76	A
ATOM	100	O	GLU	A	11	15.805	33.160	35.030	1.00	54.78	A
ATOM	101	N	ILE	A	12	15.945	31.443	33.575	1.00	52.61	A
ATOM	102	CA	ILE	A	12	15.510	32.210	32.414	1.00	50.09	A
ATOM	103	CB	ILE	A	12	16.002	31.548	31.096	1.00	50.23	A
ATOM	104	CG2	ILE	A	12	15.201	32.073	29.905	1.00	48.54	A
ATOM	105	CG1	ILE	A	12	17.508	31.773	30.930	1.00	50.30	A
ATOM	106	CD1	ILE	A	12	18.114	31.062	29.724	1.00	53.10	A
ATOM	107	C	ILE	A	12	13.988	32.324	32.362	1.00	49.83	A
ATOM	108	O	ILE	A	12	13.447	33.376	32.017	1.00	47.70	A
ATOM	109	N	GLU	A	13	13.306	31.232	32.698	1.00	48.57	A
ATOM	110	CA	GLU	A	13	11.849	31.218	32.677	1.00	48.22	A
ATOM	111	CB	GLU	A	13	11.520	29.810	32.954	1.00	45.44	A

Figure 11B

ATOM	112	CG	GLU	A	13	11.673	28.794	31.895	1.00	46.65	A
ATOM	113	CD	GLU	A	13	11.419	27.372	32.358	1.00	49.90	A
ATOM	114	OE1	GLU	A	13	12.051	26.968	33.366	1.00	49.96	A
ATOM	115	OE2	GLU	A	13	10.599	26.665	31.720	1.00	50.18	A
ATOM	116	C	GLU	A	13	11.357	32.163	33.749	1.00	47.83	A
ATOM	117	O	GLU	A	13	10.279	32.731	33.638	1.00	48.72	A
ATOM	118	N	SER	A	14	12.168	32.313	34.786	1.00	48.67	A
ATOM	119	CA	SER	A	14	11.862	33.187	35.907	1.00	49.89	A
ATOM	120	CB	SER	A	14	12.906	32.985	37.014	1.00	49.05	A
ATOM	121	OG	SER	A	14	12.634	33.773	38.160	1.00	49.35	A
ATOM	122	C	SER	A	14	11.885	34.627	35.415	1.00	50.52	A
ATOM	123	O	SER	A	14	10.869	35.313	35.431	1.00	54.15	A
ATOM	124	N	LYS	A	15	13.056	35.067	34.971	1.00	49.27	A
ATOM	125	CA	LYS	A	15	13.248	36.416	34.474	1.00	51.02	A
ATOM	126	CB	LYS	A	15	14.707	36.589	34.042	1.00	54.30	A
ATOM	127	CG	LYS	A	15	15.018	37.931	33.417	1.00	58.79	A
ATOM	128	CD	LYS	A	15	14.843	39.039	34.437	1.00	63.42	A
ATOM	129	CE	LYS	A	15	15.841	38.880	35.576	1.00	65.66	A
ATOM	130	NZ	LYS	A	15	15.722	39.983	36.569	1.00	68.14	A
ATOM	131	C	LYS	A	15	12.313	36.758	33.305	1.00	50.99	A
ATOM	132	O	LYS	A	15	12.022	37.926	33.061	1.00	49.62	A
ATOM	133	N	GLN	A	16	11.848	35.740	32.587	1.00	50.06	A
ATOM	134	CA	GLN	A	16	10.965	35.937	31.444	1.00	49.96	A
ATOM	135	CB	GLN	A	16	10.950	34.684	30.570	1.00	49.89	A
ATOM	136	CG	GLN	A	16	10.133	34.810	29.286	1.00	50.59	A
ATOM	137	CD	GLN	A	16	10.287	33.603	28.369	1.00	54.27	A
ATOM	138	OE1	GLN	A	16	9.799	32.511	28.667	1.00	56.28	A
ATOM	139	NE2	GLN	A	16	10.985	33.796	27.250	1.00	54.69	A
ATOM	140	C	GLN	A	16	9.551	36.256	31.899	1.00	50.61	A
ATOM	141	O	GLN	A	16	8.788	36.931	31.195	1.00	48.56	A
ATOM	142	N	LYS	A	17	9.198	35.736	33.067	1.00	49.38	A
ATOM	143	CA	LYS	A	17	7.883	35.973	33.623	1.00	49.73	A
ATOM	144	CB	LYS	A	17	7.582	34.982	34.750	1.00	52.97	A
ATOM	145	CG	LYS	A	17	6.250	35.226	35.448	1.00	56.86	A
ATOM	146	CD	LYS	A	17	6.066	34.276	36.618	1.00	59.31	A
ATOM	147	CE	LYS	A	17	4.763	34.552	37.354	1.00	59.95	A
ATOM	148	NZ	LYS	A	17	4.592	33.621	38.506	1.00	62.05	A
ATOM	149	C	LYS	A	17	7.927	37.390	34.163	1.00	48.25	A
ATOM	150	O	LYS	A	17	6.977	38.144	34.008	1.00	47.73	A
ATOM	151	N	LYS	A	18	9.043	37.750	34.791	1.00	45.58	A
ATOM	152	CA	LYS	A	18	9.190	39.101	35.309	1.		

Figure 11C

SECRET - 214531603

ATOM	172	CD	GLU	A	20	5.446	36.019	29.659	1.00	50.57	A
ATOM	173	OE1	GLU	A	20	5.832	35.316	30.617	1.00	52.42	A
ATOM	174	OE2	GLU	A	20	4.708	35.575	28.752	1.00	52.16	A
ATOM	175	C	GLU	A	20	5.195	40.546	31.873	1.00	40.09	A
ATOM	176	O	GLU	A	20	4.148	41.056	31.480	1.00	40.96	A
ATOM	177	N	ASN	A	21	5.637	40.694	33.119	1.00	38.83	A
ATOM	178	CA	ASN	A	21	4.880	41.498	34.071	1.00	40.69	A
ATOM	179	CB	ASN	A	21	5.216	41.107	35.507	1.00	39.42	A
ATOM	180	CG	ASN	A	21	4.518	39.768	35.892	1.00	41.35	A
ATOM	181	OD1	ASN	A	21	3.905	39.151	35.102	1.00	38.98	A
ATOM	182	ND2	ASN	A	21	4.902	39.312	37.107	1.00	40.82	A
ATOM	183	C	ASN	A	21	5.163	42.958	33.846	1.00	42.25	A
ATOM	184	O	ASN	A	21	4.261	43.801	33.872	1.00	42.61	A
ATOM	185	N	GLU	A	22	6.432	43.244	33.602	1.00	41.94	A
ATOM	186	CA	GLU	A	22	6.893	44.589	33.343	1.00	41.44	A
ATOM	187	CB	GLU	A	22	8.403	44.563	33.127	1.00	43.01	A
ATOM	188	CG	GLU	A	22	9.126	45.861	33.421	1.00	49.75	A
ATOM	189	CD	GLU	A	22	9.769	45.872	34.802	1.00	52.80	A
ATOM	190	OE1	GLU	A	22	10.611	44.988	35.077	1.00	53.66	A
ATOM	191	OE2	GLU	A	22	9.447	46.764	35.608	1.00	57.41	A
ATOM	192	C	GLU	A	22	6.188	45.082	32.068	1.00	41.34	A
ATOM	193	O	GLU	A	22	5.851	46.263	31.954	1.00	43.52	A
ATOM	194	N	ILE	A	23	5.964	44.175	31.116	1.00	37.55	A
ATOM	195	CA	ILE	A	23	5.295	44.530	29.863	1.00	35.10	A
ATOM	196	CB	ILE	A	23	5.418	43.408	28.800	1.00	36.19	A
ATOM	197	CG2	ILE	A	23	4.520	43.719	27.592	1.00	35.94	A
ATOM	198	CG1	ILE	A	23	6.876	43.288	28.340	1.00	39.18	A
ATOM	199	CD1	ILE	A	23	7.122	42.193	27.324	1.00	40.80	A
ATOM	200	C	ILE	A	23	3.816	44.827	30.093	1.00	32.36	A
ATOM	201	O	ILE	A	23	3.284	45.796	29.568	1.00	28.55	A
ATOM	202	N	ALA	A	24	3.167	43.981	30.881	1.00	30.41	A
ATOM	203	CA	ALA	A	24	1.760	44.147	31.179	1.00	30.11	A
ATOM	204	CB	ALA	A	24	1.276	42.994	32.043	1.00	27.29	A
ATOM	205	C	ALA	A	24	1.531	45.479	31.893	1.00	31.41	A
ATOM	206	O	ALA	A	24	0.562	46.183	31.608	1.00	31.49	A
ATOM	207	N	ARG	A	25	2.428	45.825	32.816	1.00	30.94	A
ATOM	208	CA	ARG	A	25	2.297	47.070	33.547	1.00	30.44	A
ATOM	209	CB	ARG	A	25	3.197	47.066	34.798	1.00	32.01	A
ATOM	210	CG	ARG	A	25	2.727	46.101	35.894	1.00	34.49	A
ATOM	211	CD	ARG	A	25	3.471	46.326	37.218	1.00	39.65	A
ATOM	212	NE	ARG	A	25	4.873	45.907	37.177	1.00	40.74	A
ATOM	213	CZ	ARG	A	25	5.308	44.687	37.496	1.00	43.06	A
ATOM	214	NH1	ARG	A	25	4.453	43.749	37.885	1.00	39.85	A
ATOM	215	NH2	ARG	A	25	6.606	44.399	37.399	1.00	40.30	A
ATOM	216	C	ARG	A	25	2.590	48.270	32.651	1.00	28.86	A
ATOM	217	O	ARG	A	25	1.907	49.296	32.728	1.00	29.35	A
ATOM	218	N	ILE	A	26	3.587	48.147	31.790	1.00	26.96	A
ATOM	219	CA	ILE	A	26	3.917	49.226	30.875	1.00	29.07	A
ATOM	220	CB	ILE	A	26	5.132	48.832	29.990	1.00	28.43	A
ATOM	221	CG2	ILE	A	26	5.239	49.760	28.799	1.00	25.38	A
ATOM	222	CG1	ILE	A	26	6.414	48.835	30.839	1.00	28.70	A
ATOM	223	CD1	ILE	A	26	7.646	48.257	30.132	1.00	27.77	A
ATOM	224	C	ILE	A	26	2.719	49.571	29.968	1.00	30.92	A
ATOM	225	O	ILE	A	26	2.435	50.746	29.690	1.00	32.33	A
ATOM	226	N	LYS	A	27	2.019	48.540	29.512	1.00	30.36	A
ATOM	227	CA	LYS	A	27	0.887	48.730	28.627	1.00	30.40	A
ATOM	228	CB	LYS	A	27	0.449	47.388	28.045	1.00	33.83	A
ATOM	229	CG	LYS	A	27	1.520	46.729	27.185	1.00	39.64	A
ATOM	230	CD	LYS	A	27	1.167	45.294	26.831	1.00	44.41	A
ATOM	231	CE	LYS	A	27	-0.086	45.204	26.003	1.00	46.84	A

Figure 11D

ATOM	232	NZ	LYS	A	27	-0.384	43.774	25.698	1.00	53.94	A
ATOM	233	C	LYS	A	27	-0.267	49.402	29.344	1.00	38.67	A
ATOM	234	O	LYS	A	27	-0.919	50.252	28.767	1.00	26.05	A
ATOM	235	N	LYS	A	28	-0.511	49.020	30.593	1.00	27.68	A
ATOM	236	CA	LYS	A	28	-1.597	49.609	31.371	1.00	27.30	A
ATOM	237	CB	LYS	A	28	-1.797	48.845	32.691	1.00	24.82	A
ATOM	238	CG	LYS	A	28	-2.961	49.384	33.573	1.00	27.48	A
ATOM	239	CD	LYS	A	28	-4.263	49.506	32.744	1.00	31.59	A
ATOM	240	CE	LYS	A	28	-5.526	49.699	33.606	1.00	30.02	A
ATOM	241	NZ	LYS	A	28	-5.440	50.820	34.586	1.00	31.11	A
ATOM	242	C	LYS	A	28	-1.284	51.076	31.641	1.00	29.57	A
ATOM	243	O	LYS	A	28	-2.164	51.951	31.566	1.00	28.21	A
ATOM	244	N	LEU	A	29	-0.017	51.359	31.923	1.00	29.36	A
ATOM	245	CA	LEU	A	29	0.385	52.723	32.179	1.00	33.70	A
ATOM	246	CB	LEU	A	29	1.822	52.745	32.692	1.00	35.26	A
ATOM	247	CG	LEU	A	29	2.023	53.727	33.847	1.00	38.04	A
ATOM	248	CD1	LEU	A	29	3.363	53.485	34.506	1.00	39.85	A
ATOM	249	CD2	LEU	A	29	1.891	55.149	33.332	1.00	38.01	A
ATOM	250	C	LEU	A	29	0.243	53.561	30.905	1.00	34.59	A
ATOM	251	O	LEU	A	29	-0.281	54.691	30.927	1.00	37.16	A
ATOM	252	N	LEU	A	30	0.721	53.020	29.792	1.00	34.03	A
ATOM	253	CA	LEU	A	30	0.616	53.724	28.528	1.00	35.56	A
ATOM	254	CB	LEU	A	30	1.230	52.874	27.414	1.00	38.09	A
ATOM	255	CG	LEU	A	30	1.470	53.508	26.050	1.00	40.19	A
ATOM	256	CD1	LEU	A	30	2.270	54.805	26.163	1.00	39.79	A
ATOM	257	CD2	LEU	A	30	2.215	52.484	25.198	1.00	45.44	A
ATOM	258	C	LEU	A	30	-0.882	53.980	28.263	1.00	34.76	A
ATOM	259	O	LEU	A	30	-1.269	55.050	27.794	1.00	33.56	A
ATOM	260	N	GLN	A	31	-1.713	52.996	28.572	1.00	30.55	A
ATOM	261	CA	GLN	A	31	-3.152	53.142	28.401	1.00	31.04	A
ATOM	262	CB	GLN	A	31	-3.865	51.839	28.782	1.00	33.01	A
ATOM	263	CG	GLN	A	31	-5.397	51.924	28.839	1.00	37.09	A
ATOM	264	CD	GLN	A	31	-6.045	50.582	29.159	1.00	45.53	A
ATOM	265	OE1	GLN	A	31	-5.715	49.940	30.159	1.00	52.72	A
ATOM	266	NE2	GLN	A	31	-6.973	50.151	28.310	1.00	46.91	A
ATOM	267	C	GLN	A	31	-3.633	54.303	29.273	1.00	31.34	A
ATOM	268	O	GLN	A	31	-4.419	55.125	28.832	1.00	28.45	A
ATOM	269	N	LEU	A	32	-3.141	54.376	30.509	1.00	30.93	A
ATOM	270	CA	LEU	A	32	-3.523	55.459	31.393	1.00	30.83	A
ATOM	271	CB	LEU	A	32	-2.988	55.237	32.811	1.00	29.49	A
ATOM	272	CG	LEU	A	32	-3.572	54.156	33.732	1.00	31.79	A
ATOM	273	CD1	LEU	A	32	-2.810	54.215	35.075	1.00	33.29	A
ATOM	274	CD2	LEU	A	32	-5.058	54.376	33.972	1.00	25.39	A
ATOM	275	C	LEU	A	32	-3.031	56.797	30.860	1.00	32.26	A
ATOM	276	O	LEU	A	32	-3.707	57.810	31.031	1.00	35.77	A
ATOM	277	N	THR	A	33	-1.872	56.798	30.198	1.00	31.70	A
ATOM	278	CA	THR	A	33	-1.298	58.019	29.640	1.00	33.33	A
ATOM	279	CB	THR	A	33	0.158	57.787	29.156	1.00	35.07	A
ATOM	280	OG1	THR	A	33	0.949	57.272	30.238	1.00	39.00	A
ATOM	281	CG2	THR	A	33	0.776	59.087	28.687	1.00	34.58	A
ATOM	282	C	THR	A	33	-2.120	58.560	28.471	1.00	33.63	A
ATOM	283	O	THR	A	33	-2.237	59.767	28.298	1.00	33.87	A
ATOM	284	N	VAL	A	34	-2.682	57.660	27.670	1.00	35.32	A
ATOM	285	CA	VAL	A	34	-3.507	58.046	26.531	1.00	36.90	A
ATOM	286	CB	VAL	A	34	-3.810	56.832	25.622	1.00	36.47	A
ATOM	287	CG1	VAL	A	34	-4.825	57.200	24.550	1.00	34.36	A
ATOM	288	CG2	VAL	A	34	-2.514	56.354	24.966	1.00	38.97	A
ATOM	289	C	VAL	A	34	-4.809	58.655	27.036	1.00	37.01	A
ATOM	290	O	VAL	A	34	-5.250	59.695	26.540	1.00	35.59	A
ATOM	291	N	TRP	A	35	-5.403	57.992	28.022	1.00	36.34	A

Figure 11E

Figure 11F

ATOM	352	N	ALA	A	42	-9.971	67.722	26.679	1.00	67.16	A
ATOM	353	CA	ALA	A	42	-11.362	68.150	26.693	1.00	70.08	A
ATOM	354	CB	ALA	A	42	-12.352	67.043	27.249	1.00	68.59	A
ATOM	355	C	ALA	A	42	-11.461	69.423	27.556	1.00	72.76	A
ATOM	356	O	ALA	A	42	-12.506	69.748	28.123	1.00	73.45	A
ATOM	357	N	ARG	A	43	-10.338	70.137	27.642	1.00	75.35	A
ATOM	358	CA	ARG	A	43	-10.202	71.377	28.413	1.00	76.97	A
ATOM	359	CB	ARG	A	43	-9.391	71.121	29.705	1.00	77.23	A
ATOM	360	CG	ARG	A	43	-10.130	70.250	30.753	1.00	77.83	A
ATOM	361	CD	ARG	A	43	-9.265	69.690	31.889	1.00	76.18	A
ATOM	362	NE	ARG	A	43	-10.053	68.919	32.864	1.00	76.19	A
ATOM	363	CZ	ARG	A	43	-10.933	67.967	32.551	1.00	76.17	A
ATOM	364	NH1	ARG	A	43	-11.153	67.657	31.284	1.00	76.24	A
ATOM	365	NH2	ARG	A	43	-11.605	67.326	33.507	1.00	77.89	A
ATOM	366	C	ARG	A	43	-9.560	72.481	27.570	1.00	79.19	A
ATOM	367	O	ARG	A	43	-10.131	72.882	26.548	1.00	79.42	A
ATOM	368	N	ILE	A	44	-8.381	72.970	27.993	1.00	81.42	A
ATOM	369	CA	ILE	A	44	-7.646	74.059	27.276	1.00	84.32	A
ATOM	370	CB	ILE	A	44	-6.073	73.998	27.495	1.00	84.97	A
ATOM	371	CG2	ILE	A	44	-5.292	74.824	26.419	1.00	85.80	A
ATOM	372	CG1	ILE	A	44	-5.728	74.612	28.829	1.00	85.52	A
ATOM	373	CD1	ILE	A	44	-6.344	76.011	29.055	1.00	87.04	A
ATOM	374	C	ILE	A	44	-7.908	73.987	25.790	1.00	86.80	A
ATOM	375	O	ILE	A	44	-8.577	74.829	25.234	1.00	87.60	A
ATOM	376	N	LEU	A	45	-7.318	73.007	25.145	1.00	87.99	A
ATOM	377	CA	LEU	A	45	-7.541	72.910	23.737	1.00	88.13	A
ATOM	378	CB	LEU	A	45	-6.257	72.509	23.009	1.00	88.79	A
ATOM	379	CG	LEU	A	45	-5.940	73.339	21.770	1.00	90.46	A
ATOM	380	CD1	LEU	A	45	-7.147	73.370	20.837	1.00	91.58	A
ATOM	381	CD2	LEU	A	45	-5.596	74.779	22.173	1.00	90.84	A
ATOM	382	C	LEU	A	45	-8.656	71.944	23.376	1.00	88.30	A
ATOM	383	O	LEU	A	45	-9.507	71.665	24.291	1.00	87.82	A
ATOM	384	NT	LEU	A	45	-8.614	71.561	22.151	1.00	88.77	A
ATOM	385	CA	ACE	B	0	29.175	18.175	21.874	1.00	35.90	B
ATOM	386	C	ACE	B	0	27.867	18.849	22.146	1.00	36.69	B
ATOM	387	O	ACE	B	0	27.836	20.078	22.299	1.00	33.24	B
ATOM	388	N	ARG	B	1	26.771	18.065	22.218	1.00	32.69	B
ATOM	389	CA	ARG	B	1	25.440	18.590	22.450	1.00	34.24	B
ATOM	390	CB	ARG	B	1	24.436	17.446	22.644	1.00	33.49	B
ATOM	391	CG	ARG	B	1	22.976	17.878	22.651	1.00	32.92	B
ATOM	392	CD	ARG	B	1	22.436	18.177	21.260	1.00	34.95	B
ATOM	393										

Figure 11G

Figure 11H

Figure 111

DEBRA M. ECKERT

ATOM	532	NZ	LYS	B	17	25.465	42.963	29.625	1.00	67.09	B
ATOM	533	C	LYS	B	17	19.389	42.522	28.230	1.00	59.16	B
ATOM	534	O	LYS	B	17	19.088	43.634	28.656	1.00	55.77	B
ATOM	535	N	LYS	B	18	19.433	42.233	26.931	1.00	58.38	B
ATOM	536	CA	LYS	B	18	19.128	43.248	25.931	1.00	58.35	B
ATOM	537	CB	LYS	B	18	19.247	42.675	24.511	1.00	59.38	B
ATOM	538	CG	LYS	B	18	20.617	42.083	24.130	1.00	61.47	B
ATOM	539	CD	LYS	B	18	21.768	43.111	24.099	1.00	61.91	B
ATOM	540	CE	LYS	B	18	22.034	43.761	25.461	1.00	63.50	B
ATOM	541	NZ	LYS	B	18	23.248	44.620	25.423	1.00	63.66	B
ATOM	542	C	LYS	B	18	17.706	43.761	26.163	1.00	58.27	B
ATOM	543	O	LYS	B	18	17.475	44.969	26.254	1.00	58.82	B
ATOM	544	N	ILE	B	19	16.757	42.835	26.268	1.00	56.89	B
ATOM	545	CA	ILE	B	19	15.356	43.189	26.488	1.00	53.76	B
ATOM	546	CB	ILE	B	19	14.455	41.931	26.488	1.00	53.33	B
ATOM	547	CG2	ILE	B	19	13.057	42.286	26.976	1.00	52.66	B
ATOM	548	CG1	ILE	B	19	14.416	41.322	25.081	1.00	52.79	B
ATOM	549	CD1	ILE	B	19	13.543	40.069	24.970	1.00	54.45	B
ATOM	550	C	ILE	B	19	15.117	43.961	27.786	1.00	52.88	B
ATOM	551	O	ILE	B	19	14.327	44.897	27.809	1.00	51.74	B
ATOM	552	N	GLU	B	20	15.781	43.565	28.869	1.00	51.04	B
ATOM	553	CA	GLU	B	20	15.601	44.267	30.128	1.00	50.08	B
ATOM	554	CB	GLU	B	20	16.403	43.613	31.253	1.00	49.90	B
ATOM	555	CG	GLU	B	20	15.969	42.207	31.584	1.00	54.19	B
ATOM	556	CD	GLU	B	20	16.761	41.620	32.736	1.00	55.98	B
ATOM	557	OE1	GLU	B	20	18.010	41.568	32.641	1.00	53.23	B
ATOM	558	OE2	GLU	B	20	16.127	41.215	33.735	1.00	56.20	B
ATOM	559	C	GLU	B	20	16.053	45.706	29.965	1.00	49.26	B
ATOM	560	O	GLU	B	20	15.479	46.611	30.561	1.00	48.88	B
ATOM	561	N	ASN	B	21	17.093	45.912	29.163	1.00	49.15	B
ATOM	562	CA	ASN	B	21	17.596	47.256	28.930	1.00	49.99	B
ATOM	563	CB	ASN	B	21	18.885	47.229	28.098	1.00	51.35	B
ATOM	564	CG	ASN	B	21	20.054	46.576	28.834	1.00	54.79	B
ATOM	565	OD1	ASN	B	21	20.421	46.978	29.943	1.00	55.96	B
ATOM	566	ND2	ASN	B	21	20.656	45.572	28.205	1.00	57.15	B
ATOM	567	C	ASN	B	21	16.537	48.078	28.202	1.00	49.83	B
ATOM	568	O	ASN	B	21	16.249	49.209	28.591	1.00	50.14	B
ATOM	569	N	GLU	B	22	15.957	47.497	27.153	1.00	47.34	B
ATOM	570	CA	GLU	B	22	14.942	48.160	26.354	1.00	44.99	B
ATOM	571	CB	GLU	B	22	14.534	47.272	25.174	1.00	44.99	B
ATOM	572	CG	GLU	B	22	13.703	47.990	24.116	1.00	51.85	B
ATOM	573	CD	GLU	B	22	14.377	49.268	23.621	1.00	54.71	B
ATOM	574	OE1	GLU	B	22	15.543	49.191	23.182	1.00	55.60	B
ATOM	575	OE2	GLU	B	22	13.743	50.350	23.673	1.00	57.01	B
ATOM	576	C	GLU	B	22	13.710	48.521	27.183	1.00	44.17	B
ATOM	577	O	GLU	B	22	13.044	49.527	26.916	1.00	45.50	B
ATOM	578	N	ILE	B	23	13.386	47.693	28.169	1.00	42.28	B
ATOM	579	CA	ILE	B	23	12.241	47.977	29.024	1.00	40.61	B
ATOM	580	CB	ILE	B	23	11.801	46.724	29.809	1.00	38.57	B
ATOM	581	CG2	ILE	B	23	10.836	47.096	30.925	1.00	37.31	B
ATOM	582	CG1	ILE	B	23	11.138	45.733	28.850	1.00	38.28	B
ATOM	583	CD1	ILE	B	23	10.634	44.436	29.530	1.00	38.32	B
ATOM	584	C	ILE	B	23	12.626	49.108	29.974	1.00	41.50	B
ATOM	585	O	ILE	B	23	11.793	49.926	30.349	1.00	41.54	B
ATOM	586	N	ALA	B	24	13.898	49.170	30.348	1.00	40.42	B
ATOM	587	CA	ALA	B	24	14.349	50.240	31.224	1.00	38.49	B
ATOM	588	CB	ALA	B	24	15.811	50.059	31.578	1.00	34.26	B
ATOM	589	C	ALA	B	24	14.147	51.562	30.490	1.00	37.76	B
ATOM	590	O	ALA	B	24	13.674	52.528	31.078	1.00	38.39	B
ATOM	591	N	ARG	B	25	14.498	51.591	29.204	1.00	36.47	B

Figure 11J

ATOM	712	CB	GLN	B	39	4.629	69.583	34.197	1.00	33.05	B
ATOM	713	CG	GLN	B	39	5.436	70.614	34.985	1.00	43.49	B
ATOM	714	CD	GLN	B	39	4.822	72.026	35.008	1.00	48.65	B
ATOM	715	OE1	GLN	B	39	4.889	72.774	34.021	1.00	51.46	B
ATOM	716	NE2	GLN	B	39	4.220	72.389	36.143	1.00	47.35	B
ATOM	717	C	GLN	B	39	2.343	70.417	33.843	1.00	31.81	B
ATOM	718	O	GLN	B	39	2.125	71.574	34.206	1.00	31.08	B
ATOM	719	N	LEU	B	40	1.897	69.904	32.703	1.00	31.01	B
ATOM	720	CA	LEU	B	40	1.065	70.671	31.807	1.00	33.41	B
ATOM	721	CB	LEU	B	40	0.872	69.886	30.517	1.00	32.63	B
ATOM	722	CG	LEU	B	40	-0.126	70.405	29.482	1.00	34.65	B
ATOM	723	CD1	LEU	B	40	0.171	71.843	29.092	1.00	35.24	B
ATOM	724	CD2	LEU	B	40	-0.058	69.495	28.281	1.00	35.90	B
ATOM	725	C	LEU	B	40	-0.289	70.943	32.469	1.00	36.85	B
ATOM	726	O	LEU	B	40	-0.874	72.010	32.314	1.00	37.81	B
ATOM	727	N	GLN	B	41	-0.768	69.964	33.215	1.00	36.13	B
ATOM	728	CA	GLN	B	41	-2.046	70.063	33.894	1.00	37.74	B
ATOM	729	CB	GLN	B	41	-2.369	68.718	34.517	1.00	41.31	B
ATOM	730	CG	GLN	B	41	-3.833	68.459	34.735	1.00	47.08	B
ATOM	731	CD	GLN	B	41	-4.070	67.139	35.420	1.00	54.09	B
ATOM	732	OE1	GLN	B	41	-3.517	66.102	35.013	1.00	55.42	B
ATOM	733	NE2	GLN	B	41	-4.908	67.154	36.461	1.00	54.90	B
ATOM	734	C	GLN	B	41	-2.039	71.148	34.974	1.00	39.95	B
ATOM	735	O	GLN	B	41	-2.988	71.925	35.089	1.00	29.23	B
ATOM	736	N	ALA	B	42	-0.972	71.194	35.767	1.00	39.05	B
ATOM	737	CA	ALA	B	42	-0.845	72.188	36.824	1.00	38.56	B
ATOM	738	CB	ALA	B	42	0.345	71.852	37.757	1.00	34.14	B
ATOM	739	C	ALA	B	42	-0.647	73.566	36.228	1.00	40.18	B
ATOM	740	O	ALA	B	42	-1.139	74.560	36.765	1.00	41.44	B
ATOM	741	N	ARG	B	43	0.078	73.634	35.118	1.00	41.82	B
ATOM	742	CA	ARG	B	43	0.340	74.910	34.476	1.00	43.71	B
ATOM	743	CB	ARG	B	43	1.242	74.713	33.260	1.00	47.26	B
ATOM	744	CG	ARG	B	43	1.703	75.997	32.592	1.00	51.08	B
ATOM	745	CD	ARG	B	43	2.582	75.677	31.401	1.00	54.95	B
ATOM	746	NE	ARG	B	43	3.778	74.947	31.813	1.00	57.04	B
ATOM	747	CZ	ARG	B	43	4.819	75.499	32.428	1.00	56.95	B
ATOM	748	NH1	ARG	B	43	4.816	76.794	32.703	1.00	55.89	B
ATOM	749	NH2	ARG	B	43	5.858	74.753	32.781	1.00	57.00	B
ATOM	750	C	ARG	B	43	-0.987	75.521	34.048	1.00	42.38	B
ATOM	751	O	ARG	B	43	-1.308	76.657	34.398	1.00	41.41	B
ATOM	752	N	ILE	B	44	-1.756	74.736	33.310	1.00	41.63	B
ATOM	753	CA	ILE	B	44	-3.059	75.143	32.810	1.00	43.24	B
ATOM	754	CB	ILE	B	44	-3.634	74.085	31.866	1.00	44.23	B
ATOM	755	CG2	ILE	B	44	-5.083	74.403	31.592	1.00	45.04	B
ATOM	756	CG1	ILE	B	44	-2.778	73.964	30.600	1.00	47.45	B
ATOM	757	CD1	ILE	B	44	-3.156	72.745	29.719	1.00	49.42	B
ATOM	758	C	ILE	B	44	-4.081	75.306	33.935	1.00	42.37	B
ATOM	759	O	ILE	B	44	-4.422	76.416	34.332	1.00	42.08	B
ATOM	760	N	LEU	B	45	-4.573	74.162	34.398	1.00	42.20	B
ATOM	761	CA	LEU	B	45	-5.564	74.042	35.450	1.00	43.16	B
ATOM	762	CB	LEU	B	45	-6.041	72.592	35.513	1.00	46.08	B
ATOM	763	CG	LEU	B	45	-6.459	72.001	34.162	1.00	47.45	B
ATOM	764	CD1	LEU	B	45	-7.011	70.594	34.257	1.00	47.51	B
ATOM	765	CD2	LEU	B	45	-7.504	72.899	33.521	1.00	48.61	B
ATOM	766	C	LEU	B	45	-5.016	74.467	36.810	1.00	42.48	B
ATOM	767	O	LEU	B	45	-5.674	75.260	37.483	1.00	45.15	B
ATOM	768	NT	LEU	B	45	-3.945	73.987	37.206	1.00	45.66	B
ATOM	769	CA	ACE	C	0	15.143	11.286	26.819	1.00	82.49	C
ATOM	770	C	ACE	C	0	14.856	12.476	27.674	1.00	82.44	C
ATOM	771	O	ACE	C	0	13.700	12.858	27.851	1.00	94.06	C

Figure 11M

001221" 031231200

ATOM	772	N	ARG	C	1	15.890	13.103	28.220	1.00	82.91	C
ATOM	773	CA	ARG	C	1	15.663	14.253	29.073	1.00	83.87	C
ATOM	774	CB	ARG	C	1	16.156	13.970	30.491	1.00	83.74	C
ATOM	775	CG	ARG	C	1	15.769	15.065	31.456	1.00	83.47	C
ATOM	776	CD	ARG	C	1	14.340	15.542	31.156	1.00	81.66	C
ATOM	777	NE	ARG	C	1	13.249	14.748	31.726	1.00	81.00	C
ATOM	778	CZ	ARG	C	1	13.069	13.434	31.597	1.00	79.16	C
ATOM	779	NH1	ARG	C	1	13.901	12.678	30.889	1.00	79.80	C
ATOM	780	NH2	ARG	C	1	12.010	12.875	32.168	1.00	79.18	C
ATOM	781	C	ARG	C	1	16.282	15.541	28.550	1.00	85.03	C
ATOM	782	O	ARG	C	1	15.975	16.644	29.016	1.00	85.10	C
ATOM	783	N	MET	C	2	17.169	15.394	27.581	1.00	85.40	C
ATOM	784	CA	MET	C	2	17.778	16.568	27.012	1.00	86.91	C
ATOM	785	CB	MET	C	2	19.063	16.215	26.290	1.00	88.20	C
ATOM	786	CG	MET	C	2	19.711	17.410	25.653	1.00	89.72	C
ATOM	787	SD	MET	C	2	21.192	16.917	24.823	1.00	94.98	C
ATOM	788	CE	MET	C	2	22.111	16.349	26.176	1.00	91.53	C
ATOM	789	C	MET	C	2	16.771	17.154	26.036	1.00	87.44	C
ATOM	790	O	MET	C	2	16.699	18.368	25.872	1.00	89.05	C
ATOM	791	N	LYS	C	3	16.001	16.278	25.391	1.00	85.66	C
ATOM	792	CA	LYS	C	3	14.973	16.712	24.444	1.00	83.09	C
ATOM	793	CB	LYS	C	3	14.033	15.551	24.107	1.00	82.50	C
ATOM	794	CG	LYS	C	3	12.921	15.895	23.122	1.00	81.54	C
ATOM	795	CD	LYS	C	3	11.926	14.746	23.005	1.00	81.93	C
ATOM	796	CE	LYS	C	3	10.866	15.022	21.952	1.00	80.79	C
ATOM	797	NZ	LYS	C	3	10.154	16.300	22.214	1.00	82.56	C
ATOM	798	C	LYS	C	3	14.177	17.809	25.128	1.00	82.12	C
ATOM	799	O	LYS	C	3	14.053	18.925	24.617	1.00	81.76	C
ATOM	800	N	GLN	C	4	13.651	17.474	26.302	1.00	80.32	C
ATOM	801	CA	GLN	C	4	12.856	18.401	27.094	1.00	78.87	C
ATOM	802	CB	GLN	C	4	12.504	17.759	28.440	1.00	79.91	C
ATOM	803	CG	GLN	C	4	12.122	16.275	28.356	1.00	80.66	C
ATOM	804	CD	GLN	C	4	11.087	15.971	27.280	1.00	81.02	C
ATOM	805	OE1	GLN	C	4	11.348	16.140	26.082	1.00	79.52	C
ATOM	806	NE2	GLN	C	4	9.907	15.516	27.701	1.00	81.57	C
ATOM	807	C	GLN	C	4	13.667	19.680	27.299	1.00	77.97	C
ATOM	808	O	GLN	C	4	13.186	20.781	27.032	1.00	78.45	C
ATOM	809	N	ILE	C	5	14.902	19.530	27.772	1.00	76.07	C
ATOM	810	CA	ILE	C	5	15.785	20.670	27.974	1.00	73.89	C
ATOM	811	CB	ILE	C	5	17.206	20.220	28.381	1.00	73.07	C
ATOM	812	CG2	ILE	C	5	18.175	21.388	28.264	1.00	71.17	C
ATOM	813	CG1	ILE	C	5	17.174	19.623	29.795	1.00	72.84	C
ATOM	814	CD1	ILE	C	5	18.518	19.113	30.285	1.00	71.39	C
ATOM	815	C	ILE	C	5	15.880	21.423	26.656	1.00	74.14	C
ATOM	816	O	ILE	C	5	15.939	22.651	26.628	1.00	73.70	C
ATOM	817	N	GLU	C	6	15.895	20.664	25.567	1.00	73.88	C
ATOM	818	CA	GLU	C	6	15.972	21.222	24.225	1.00	73.70	C
ATOM	819	CB	GLU	C	6	16.395	20.135	23.229	1.00	72.24	C
ATOM	820	CG	GLU	C	6	17.787	19.535	23.464	1.00	69.96	C
ATOM	821	CD	GLU	C	6	18.922	20.428	22.985	1.00	68.01	C
ATOM	822	OE1	GLU	C	6	19.044	21.575	23.461	1.00	65.93	C
ATOM	823	OE2	GLU	C	6	19.702	19.963	22.125	1.00	68.18	C
ATOM	824	C	GLU	C	6	14.602	21.773	23.842	1.00	74.50	C
ATOM	825	O	GLU	C	6	14.476	22.546	22.890	1.00	75.27	C
ATOM	826	N	ASP	C	7	13.577	21.372	24.587	1.00	74.82	C
ATOM	827	CA	ASP	C	7	12.218	21.838	24.327	1.00	76.17	C
ATOM	828	CB	ASP	C	7	11.195	20.742	24.644	1.00	77.40	C
ATOM	829	CG	ASP	C	7	11.408	19.488	23.818	1.00	78.45	C
ATOM	930	OD1	ASP	C	7	11.518	19.609	22.580	1.00	79.26	C
ATOM	931	OD2	ASP	C	7	11.452	18.380	24.404	1.00	79.10	C

Figure 11N

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ATOM	892	N	LYS	C	15	8.632	22.671	23.091	1.00	62.79	C
ATOM	893	CA	LYS	C	15	8.153	33.873	23.771	1.00	64.30	C
ATOM	894	CB	LYS	C	15	7.949	33.612	25.273	1.00	65.74	C
ATOM	895	CG	LYS	C	15	6.637	32.903	25.642	1.00	68.25	C
ATOM	896	CD	LYS	C	15	6.534	32.695	27.154	1.00	69.92	C
ATOM	897	CE	LYS	C	15	5.186	32.131	27.564	1.00	70.69	C
ATOM	898	NZ	LYS	C	15	4.078	33.079	27.241	1.00	73.69	C
ATOM	899	C	LYS	C	15	9.130	35.029	23.601	1.00	64.03	C
ATOM	900	O	LYS	C	15	8.723	36.175	23.408	1.00	64.04	C
ATOM	901	N	GLN	C	16	10.418	34.721	23.678	1.00	63.47	C
ATOM	902	CA	GLN	C	16	11.451	35.733	23.537	1.00	65.82	C
ATOM	903	CB	GLN	C	16	12.813	35.064	23.393	1.00	65.17	C
ATOM	904	CG	GLN	C	16	13.970	36.027	23.413	1.00	65.29	C
ATOM	905	CD	GLN	C	16	14.944	35.695	24.516	1.00	66.93	C
ATOM	906	OE1	GLN	C	16	15.940	36.389	24.719	1.00	68.97	C
ATOM	907	NE2	GLN	C	16	14.657	34.621	25.244	1.00	66.55	C
ATOM	908	C	GLN	C	16	11.157	36.605	22.317	1.00	67.53	C
ATOM	909	O	GLN	C	16	11.172	37.836	22.397	1.00	68.90	C
ATOM	910	N	LYS	C	17	10.886	35.952	21.193	1.00	67.63	C
ATOM	911	CA	LYS	C	17	10.566	36.648	19.954	1.00	67.83	C
ATOM	912	CB	LYS	C	17	10.355	35.627	18.833	1.00	69.39	C
ATOM	913	CG	LYS	C	17	9.747	36.199	17.556	1.00	72.05	C
ATOM	914	CD	LYS	C	17	10.657	37.203	16.835	1.00	73.47	C
ATOM	915	CE	LYS	C	17	9.946	37.784	15.613	1.00	74.71	C
ATOM	916	NZ	LYS	C	17	10.885	38.603	14.795	1.00	76.15	C
ATOM	917	C	LYS	C	17	9.306	37.492	20.123	1.00	66.64	C
ATOM	918	O	LYS	C	17	9.244	38.632	19.652	1.00	67.45	C
ATOM	919	N	LYS	C	18	8.300	36.924	20.784	1.00	64.29	C
ATOM	920	CA	LYS	C	18	7.049	37.641	21.019	1.00	63.62	C
ATOM	921	CB	LYS	C	18	5.979	36.719	21.627	1.00	64.15	C
ATOM	922	CG	LYS	C	18	5.088	36.062	20.586	1.00	66.52	C
ATOM	923	CD	LYS	C	18	3.935	35.297	21.220	1.00	68.98	C
ATOM	924	CE	LYS	C	18	4.427	34.076	21.970	1.00	70.96	C
ATOM	925	NZ	LYS	C	18	5.098	33.116	21.040	1.00	72.62	C
ATOM	926	C	LYS	C	18	7.265	38.852	21.922	1.00	61.00	C
ATOM	927	O	LYS	C	18	6.854	39.958	21.585	1.00	61.84	C
ATOM	928	N	ILE	C	19	7.904	38.653	23.067	1.00	56.58	C
ATOM	929	CA	ILE	C	19	8.179	39.765	23.961	1.00	53.92	C
ATOM	930	CB	ILE	C	19	9.101	39.329	25.119	1.00	52.10	C
ATOM	931	CG2	ILE	C	19	9.719	40.545	25.799	1.00	51.95	C
ATOM	932	CG1	ILE	C	19	8.304	38.463	26.095	1.00	51.65	C
ATOM	933	CD1	ILE	C	19	9.103	37.908	27.247	1.00	50.93	C
ATOM	934	C	ILE	C	19	8.833	40.893	23.165	1.00	53.24	C
ATOM	935	O	ILE	C	19	8.604	42.069	23.438	1.00	52.35	C
ATOM	936	N	GLU	C	20	9.642	40.534	22.173	1.00	53.82	C
ATOM	937	CA	GLU	C	20	10.294	41.536	21.338	1.00	54.86	C
ATOM	938	CB	GLU	C	20	11.393	40.910	20.472	1.00	55.74	C
ATOM	939	CG	GLU	C	20	12.554	40.318	21.251	1.00	56.50	C
ATOM	940	CD	GLU	C	20	13.683	39.851	20.352	1.00	56.98	C
ATOM	941	OE1	GLU	C	20	13.473	38.918	19.542	1.00	56.87	C
ATOM	942	OE2	GLU	C	20	14.786	40.427	20.453	1.00	58.79	C
ATOM	943	C	GLU	C	20	9.245	42.188	20.437	1.00	55.80	C
ATOM	944	O	GLU	C	20	9.311	42.382	20.166	1.00	55.44	C
ATOM	945	N	ASN	C	21	8.289	41.389	19.972	1.00	55.46	C
ATOM	946	CA	ASN	C	21	7.223	41.899	19.118	1.00	57.62	C
ATOM	947	CB	ASN	C	21	6.392	40.754	18.530	1.00	59.92	C
ATOM	948	CG	ASN	C	21	7.060	40.101	17.325	1.00	63.29	C
ATOM	949	OD1	ASN	C	21	6.574	39.092	16.806	1.00	62.67	C
ATOM	950	ND2	ASN	C	21	8.169	40.684	16.866	1.00	61.87	C
ATOM	951	C	ASN	C	21	6.307	42.829	19.891	1.00	58.25	C

Figure 11P

ATOM	1012	N	LEU	C	29	4.275	53.138	19.671	1.00	52.27	C
ATOM	1013	CA	LEU	C	29	3.025	53.649	20.214	1.00	51.04	C
ATOM	1014	CB	LEU	C	29	2.281	52.485	20.855	1.00	51.13	C
ATOM	1015	CG	LEU	C	29	0.776	52.493	21.051	1.00	50.66	C
ATOM	1016	CD1	LEU	C	29	0.051	52.868	19.755	1.00	51.59	C
ATOM	1017	CD2	LEU	C	29	0.389	51.100	21.491	1.00	50.29	C
ATOM	1018	C	LEU	C	29	3.347	54.739	21.245	1.00	50.83	C
ATOM	1019	O	LEU	C	29	2.739	55.805	21.269	1.00	53.58	C
ATOM	1020	N	LEU	C	30	4.327	54.457	22.089	1.00	50.52	C
ATOM	1021	CA	LEU	C	30	4.767	55.397	23.100	1.00	48.88	C
ATOM	1022	CB	LEU	C	30	5.813	54.730	23.997	1.00	48.03	C
ATOM	1023	CG	LEU	C	30	6.485	55.530	25.113	1.00	47.31	C
ATOM	1024	CD1	LEU	C	30	5.447	56.172	26.033	1.00	45.24	C
ATOM	1025	CD2	LEU	C	30	7.398	54.575	25.889	1.00	48.28	C
ATOM	1026	C	LEU	C	30	5.374	56.587	22.379	1.00	48.83	C
ATOM	1027	O	LEU	C	30	5.020	57.736	22.642	1.00	48.40	C
ATOM	1028	N	GLN	C	31	6.298	56.289	21.470	1.00	49.93	C
ATOM	1029	CA	GLN	C	31	6.983	57.304	20.670	1.00	52.00	C
ATOM	1030	CB	GLN	C	31	7.822	56.609	19.590	1.00	55.56	C
ATOM	1031	CG	GLN	C	31	8.628	57.513	18.645	1.00	61.26	C
ATOM	1032	CD	GLN	C	31	9.768	58.241	19.333	1.00	64.58	C
ATOM	1033	OE1	GLN	C	31	10.233	57.818	20.391	1.00	68.00	C
ATOM	1034	NE2	GLN	C	31	10.249	59.318	18.715	1.00	64.37	C
ATOM	1035	C	GLN	C	31	5.947	58.225	20.009	1.00	49.56	C
ATOM	1036	O	GLN	C	31	6.192	59.415	19.814	1.00	45.68	C
ATOM	1037	N	LEU	C	32	4.793	57.657	19.675	1.00	47.64	C
ATOM	1038	CA	LEU	C	32	3.723	58.401	19.034	1.00	48.95	C
ATOM	1039	CB	LEU	C	32	2.689	57.433	18.461	1.00	50.72	C
ATOM	1040	CG	LEU	C	32	1.602	57.925	17.502	1.00	51.93	C
ATOM	1041	CD1	LEU	C	32	2.209	58.293	16.154	1.00	50.26	C
ATOM	1042	CD2	LEU	C	32	0.554	56.840	17.313	1.00	51.55	C
ATOM	1043	C	LEU	C	32	3.070	59.295	20.077	1.00	49.32	C
ATOM	1044	O	LEU	C	32	3.040	60.519	19.929	1.00	50.01	C
ATOM	1045	N	THR	C	33	2.545	58.659	21.125	1.00	48.74	C
ATOM	1046	CA	THR	C	33	1.878	59.324	22.246	1.00	43.86	C
ATOM	1047	CB	THR	C	33	1.643	58.329	23.400	1.00	46.04	C
ATOM	1048	OG1	THR	C	33	0.707	57.332	22.977	1.00	47.18	C
ATOM	1049	CG2	THR	C	33	1.121	59.039	24.639	1.00	42.89	C
ATOM	1050	C	THR	C	33	2.683	60.494	22.771	1.00	41.04	C
ATOM	1051	O	THR	C	33	2.132	61.537	23.122	1.00	39.26	C
ATOM	1052	N	VAL	C	34	3.992	60.303	22.843	1.00	38.83	C
ATOM	1053	CA	VAL	C	34	4.886	61.346	23.301	1.00	36.90	C
ATOM	1054	CB	VAL	C	34	6.329	60.825	23.377	1.00	33.71	C
ATOM	1055	CG1	VAL	C	34	7.270	61.907	23.904	1.00	29.40	C
ATOM	1056	CG2	VAL	C	34	6.366	59.590	24.251	1.00	31.78	C
ATOM	1057	C	VAL	C	34	4.795	62.437	22.254	1.00	38.65	C
ATOM	1058	O	VAL	C	34	4.489	63.595	22.556	1.00	39.38	C
ATOM	1059	N	TRP	C	35	5.049	62.038	21.010	1.00	42.18	C
ATOM	1060	CA	TRP	C	35	5.002	62.937	19.868	1.00	40.00	C
ATOM	1061	CB	TRP	C	35	4.991	62.134	18.563	1.00	40.06	C
ATOM	1062	CG	TRP	C	35	4.848	63.020	17.399	1.00	36.56	C
ATOM	1063	CD2	TRP	C	35	3.696	63.161	16.561	1.00	36.91	C
ATOM	1064	CE2	TRP	C	35	3.968	64.212	15.673	1.00	41.20	C
ATOM	1065	CE3	TRP	C	35	2.457	62.505	16.503	1.00	40.31	C
ATOM	1066	CD1	TRP	C	35	5.748	63.944	16.974	1.00	35.30	C
ATOM	1067	NE1	TRP	C	35	5.228	64.673	13.945	1.00	29.45	C
ATOM	1068	CE2	TRP	C	35	3.037	64.643	14.704	1.00	38.75	C
ATOM	1069	CE3	TRP	C	35	1.528	62.934	15.541	1.00	29.54	C
ATOM	1070	CH2	TRP	C	35	1.827	63.984	14.651	1.00	41.30	C
ATOM	1071	C	TRP	C	35	3.764	63.833	19.901	1.00	39.80	C

Figure 11R

Figure 11S

ATOM	1132	NH1	ARG	C	43	-5.127	70.717	19.051	1.00	41.40	C
ATOM	1133	NH2	ARG	C	43	-6.676	72.288	18.421	1.00	44.00	C
ATOM	1134	C	ARG	C	43	-0.568	75.347	21.882	1.00	37.96	C
ATOM	1135	O	ARG	C	43	-1.049	76.425	21.558	1.00	36.78	C
ATOM	1136	N	ILE	C	44	-0.434	74.971	23.151	1.00	41.66	C
ATOM	1137	CA	ILE	C	44	-0.901	75.799	24.250	1.00	43.04	C
ATOM	1138	CB	ILE	C	44	-1.403	74.891	25.390	1.00	45.88	C
ATOM	1139	CG2	ILE	C	44	-1.802	75.717	26.594	1.00	46.21	C
ATOM	1140	CG1	ILE	C	44	-2.572	74.041	24.876	1.00	46.16	C
ATOM	1141	CD1	ILE	C	44	-2.926	72.877	25.786	1.00	50.31	C
ATOM	1142	C	ILE	C	44	0.109	76.802	24.807	1.00	41.15	C
ATOM	1143	O	ILE	C	44	-0.235	77.961	25.047	1.00	40.03	C
ATOM	1144	N	LEU	C	45	1.345	76.350	25.005	1.00	40.33	C
ATOM	1145	CA	LEU	C	45	2.401	77.184	25.579	1.00	39.81	C
ATOM	1146	CB	LEU	C	45	3.357	76.322	26.422	1.00	40.22	C
ATOM	1147	CG	LEU	C	45	2.889	75.608	27.694	1.00	40.80	C
ATOM	1148	CD1	LEU	C	45	1.733	74.714	27.364	1.00	42.51	C
ATOM	1149	CD2	LEU	C	45	4.029	74.789	28.299	1.00	39.44	C
ATOM	1150	C	LEU	C	45	3.215	77.953	24.540	1.00	38.95	C
ATOM	1151	O	LEU	C	45	3.071	77.689	23.327	1.00	39.83	C
ATOM	1152	NT	LEU	C	45	4.014	78.810	24.964	1.00	39.47	C
ATOM	1153	OH2	TIP	W	2	8.280	62.369	27.138	1.00	38.82	W
ATOM	1154	OH2	TIP	W	3	28.782	24.001	17.582	1.00	78.47	W
ATOM	1155	OH2	TIP	W	4	0.492	62.209	33.896	1.00	50.43	W
ATOM	1156	OH2	TIP	W	5	6.020	70.609	23.199	1.00	45.29	W
ATOM	1157	OH2	TIP	W	6	1.993	78.695	31.896	1.00	37.25	W
ATOM	1158	OH2	TIP	W	7	20.294	18.975	19.485	1.00	49.56	W
ATOM	1159	OH2	TIP	W	8	18.592	15.442	35.405	1.00	34.86	W
ATOM	1160	OH2	TIP	W	9	-5.907	64.337	32.524	1.00	31.24	W
ATOM	1161	OH2	TIP	W	10	11.567	18.853	30.945	1.00	47.94	W
ATOM	1162	OH2	TIP	W	11	-9.321	65.456	23.794	1.00	46.60	W
ATOM	1163	OH2	TIP	W	12	-2.842	65.953	28.078	1.00	59.15	W
ATOM	1164	OH2	TIP	W	13	-1.409	77.305	18.859	1.00	37.51	W
ATOM	1165	OH2	TIP	W	14	-5.597	64.224	37.408	1.00	39.02	W
ATOM	1166	OH2	TIP	W	15	-5.079	75.908	18.460	1.00	48.65	W
ATOM	1167	OH2	TIP	W	16	12.444	58.431	21.920	1.00	62.97	W
ATOM	1168	OH2	TIP	W	17	-12.927	70.555	24.520	1.00	61.81	W
ATOM	1169	OH2	TIP	W	18	14.897	23.356	34.046	1.00	40.13	W
ATOM	1170	OH2	TIP	W	19	3.154	40.721	28.964	1.00	29.89	W
ATOM	1171	OH2	TIP	W	20	4.290	81.951	24.440	1.00	44.83	W
ATOM	1172	OH2	TIP	W	21	26.490	23.104	32.265	1.00	62.67	W
ATOM	1173	OH2	TIP	W	22	13.085	59.162	33.622	1.00	54.53	W
ATOM	1174	OH2	TIP	W	23	-0.166	45.626	35.200	1.00	56.34	W
ATOM	1175	OH2	TIP	W	24	-10.278	62.692	33.867	1.00	64.05	W
ATOM	1176	OH2	TIP	W	25	22.697	10.892	29.710	1.00	100.00	W
ATOM	1177	OH2	TIP	W	26	4.281	39.194	26.136	1.00	62.29	W
ATOM	1178	OH2	TIP	W	27	22.833	20.843	19.882	1.00	59.57	W
ATOM	1179	OH2	TIP	W	28	-10.030	74.838	23.517	1.00	53.18	W
ATOM	1180	OH2	TIP	W	29	1.246	80.456	24.973	1.00	36.18	W
ATOM	1181	OH2	TIP	W	30	-3.034	76.181	17.506	1.00	50.44	W
ATOM	1182	OH2	TIP	W	31	1.424	49.275	18.155	1.00	44.03	W
ATOM	1183	OH2	TIP	W	32	6.269	64.921	23.710	1.00	31.68	W
ATOM	1184	OH2	TIP	W	33	27.134	28.497	40.798	1.00	60.31	W
ATOM	1185	OH2	TIP	W	34	24.326	28.221	41.517	1.00	85.52	W
ATOM	1186	OH2	TIP	W	35	24.492	26.009	31.850	1.00	68.20	W
ATOM	1187	OH2	TIP	W	36	17.270	23.540	41.621	1.00	45.61	W
ATOM	1188	OH2	TIP	W	37	17.175	27.169	41.299	1.00	57.26	W
ATOM	1189	OH2	TIP	W	38	17.133	30.154	42.769	1.00	94.65	W
ATOM	1190	OH2	TIP	W	39	23.961	29.473	38.207	1.00	73.43	W
ATOM	1191	OH2	TIP	W	40	26.646	30.299	35.030	1.00	86.46	W

Figure 11T

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ATOM	1192	OH2	TIP	W	41	21.799	33.921	37.475	1.00	98.23	W
ATOM	1193	OH2	TIP	W	42	12.296	24.508	37.800	1.00	73.10	W
ATOM	1194	OH2	TIP	W	43	10.910	28.524	40.599	1.00	65.23	W
ATOM	1195	OH2	TIP	W	44	8.726	30.065	36.214	1.00	62.46	W
ATOM	1196	OH2	TIP	W	45	20.748	34.061	34.804	1.00	62.12	W
ATOM	1197	OH2	TIP	W	46	7.462	29.159	29.170	1.00	88.23	W
ATOM	1198	OH2	TIP	W	47	7.466	31.280	33.124	1.00	56.10	W
ATOM	1199	OH2	TIP	W	48	6.666	26.619	36.241	1.00	52.76	W
ATOM	1200	OH2	TIP	W	49	3.823	27.148	35.557	1.00	92.76	W
ATOM	1201	OH2	TIP	W	50	7.608	28.183	32.367	1.00	83.54	W
ATOM	1202	OH2	TIP	W	51	10.064	35.767	38.975	1.00	68.12	W
ATOM	1203	OH2	TIP	W	52	14.649	36.973	38.236	1.00	73.09	W
ATOM	1204	OH2	TIP	W	53	16.799	36.406	39.778	1.00	48.69	W
ATOM	1205	OH2	TIP	W	54	15.456	39.954	39.598	1.00	48.97	W
ATOM	1206	OH2	TIP	W	55	8.442	41.891	37.753	1.00	57.63	W
ATOM	1207	OH2	TIP	W	56	9.926	44.040	39.986	1.00	80.20	W
ATOM	1208	OH2	TIP	W	57	3.713	35.630	32.034	1.00	65.94	W
ATOM	1209	OH2	TIP	W	58	4.004	32.569	30.481	1.00	98.02	W
ATOM	1210	OH2	TIP	W	59	13.514	45.594	36.374	1.00	45.92	W
ATOM	1211	OH2	TIP	W	60	12.274	44.358	32.693	1.00	69.72	W
ATOM	1212	OH2	TIP	W	61	-1.770	41.459	30.288	1.00	86.62	W
ATOM	1213	OH2	TIP	W	62	-0.747	39.619	34.003	1.00	85.57	W
ATOM	1214	OH2	TIP	W	63	2.370	42.056	36.997	1.00	63.26	W
ATOM	1215	OH2	TIP	W	64	7.646	47.813	26.559	1.00	86.77	W
ATOM	1216	OH2	TIP	W	65	-1.942	50.096	25.818	1.00	33.47	W
ATOM	1217	OH2	TIP	W	66	-0.455	48.262	24.057	1.00	48.49	W
ATOM	1218	OH2	TIP	W	67	-1.850	44.976	32.352	1.00	46.88	W
ATOM	1219	OH2	TIP	W	68	-4.779	47.469	30.587	1.00	53.38	W
ATOM	1220	OH2	TIP	W	69	-8.800	47.417	32.155	1.00	55.34	W
ATOM	1221	OH2	TIP	W	70	-7.762	51.374	35.608	1.00	72.46	W
ATOM	1222	OH2	TIP	W	71	5.493	50.307	35.418	1.00	63.93	W
ATOM	1223	OH2	TIP	W	72	-2.293	60.557	33.176	1.00	58.13	W
ATOM	1224	OH2	TIP	W	73	-3.891	59.956	22.859	1.00	42.99	W
ATOM	1225	OH2	TIP	W	74	-2.324	52.365	23.808	1.00	68.12	W
ATOM	1226	OH2	TIP	W	75	-4.610	53.603	23.534	1.00	99.86	W
ATOM	1227	OH2	TIP	W	76	-5.369	51.351	24.806	1.00	66.59	W
ATOM	1228	OH2	TIP	W	77	-9.158	53.927	27.711	1.00	59.38	W
ATOM	1229	OH2	TIP	W	78	-6.839	60.379	22.155	1.00	48.43	W
ATOM	1230	OH2	TIP	W	79	-7.811	55.209	31.835	1.00	63.25	W
ATOM	1231	OH2	TIP	W	80	-8.988	55.740	34.680	1.00	48.03	W
ATOM	1232	OH2	TIP	W	81	-14.358	62.793	31.478	1.00	77.34	W
ATOM	1233	OH2	TIP	W	82	-14.884	67.194	30.264	1.00	100.00	W
ATOM	1234	OH2	TIP	W	83	-13.964	62.903	27.850	1.00	61.59	W
ATOM	1235	OH2	TIP	W	84	-16.467	64.338	27.598	1.00	62.99	W
ATOM	1236	OH2	TIP	W	85	-14.165	71.419	31.235	1.00	58.55	W
ATOM	1237	OH2	TIP	W	86	-12.150	75.052	20.683	1.00	54.74	W
ATOM	1238	OH2	TIP	W	87	-15.348	66.527	23.972	1.00	86.65	W
ATOM	1239	OH2	TIP	W	88	23.657	18.784	16.110	1.00	46.11	W
ATOM	1240	OH2	TIP	W	89	21.774	13.448	17.383	1.00	55.62	W
ATOM	1241	OH2	TIP	W	90	28.955	20.801	18.398	1.00	47.29	W
ATOM	1242	OH2	TIP	W	91	19.043	22.428	18.931	1.00	70.31	W
ATOM	1243	OH2	TIP	W	92	32.348	21.741	32.055	1.00	80.85	W
ATOM	1244	OH2	TIP	W	93	31.544	26.386	31.293	1.00	80.53	W
ATOM	1245	OH2	TIP	W	94	30.484	31.504	24.099	1.00	51.19	W
ATOM	1246	OH2	TIP	W	95	28.981	30.812	18.458	1.00	98.45	W
ATOM	1247	OH2	TIP	W	96	25.233	35.680	28.569	1.00	53.47	W
ATOM	1248	OH2	TIP	W	97	25.740	37.432	31.266	1.00	96.40	W
ATOM	1249	OH2	TIP	W	98	18.343	27.853	17.008	1.00	87.39	W
ATOM	1250	OH2	TIP	W	99	26.162	40.002	24.887	1.00	63.29	W
ATOM	1251	OH2	TIP	W	100	18.896	37.649	32.149	1.00	75.85	W

Figure 11U

001001-001000

ATOM	1252	OH2	TIP	W	101	20.897	31.301	18.264	1.00	88.40	W
ATOM	1253	OH2	TIP	W	102	19.191	42.582	21.453	1.00	55.18	W
ATOM	1254	OH2	TIP	W	103	23.958	41.188	26.907	1.00	78.30	W
ATOM	1255	OH2	TIP	W	104	18.433	46.716	22.932	1.00	54.59	W
ATOM	1256	OH2	TIP	W	105	22.353	48.547	25.042	1.00	59.94	W
ATOM	1257	OH2	TIP	W	106	21.797	41.049	34.496	1.00	78.60	W
ATOM	1258	OH2	TIP	W	107	21.437	46.210	33.535	1.00	75.53	W
ATOM	1259	OH2	TIP	W	108	14.907	43.959	21.380	1.00	54.65	W
ATOM	1260	OH2	TIP	W	109	15.635	42.456	19.119	1.00	58.03	W
ATOM	1261	OH2	TIP	W	110	19.533	44.310	33.666	1.00	80.58	W
ATOM	1262	OH2	TIP	W	111	18.747	50.736	29.399	1.00	60.97	W
ATOM	1263	OH2	TIP	W	112	21.131	52.757	28.680	1.00	55.70	W
ATOM	1264	OH2	TIP	W	113	17.303	55.311	38.133	1.00	72.59	W
ATOM	1265	OH2	TIP	W	114	18.939	58.215	28.845	1.00	79.75	W
ATOM	1266	OH2	TIP	W	115	14.666	59.680	28.964	1.00	50.64	W
ATOM	1267	OH2	TIP	W	116	17.408	62.649	28.523	1.00	74.43	W
ATOM	1268	OH2	TIP	W	117	12.106	61.533	23.810	1.00	89.64	W
ATOM	1269	OH2	TIP	W	118	10.138	60.131	37.626	1.00	89.60	W
ATOM	1270	OH2	TIP	W	119	14.125	60.999	36.831	1.00	78.03	W
ATOM	1271	OH2	TIP	W	120	6.987	65.584	27.400	1.00	63.28	W
ATOM	1272	OH2	TIP	W	121	8.699	65.761	30.950	1.00	64.96	W
ATOM	1273	OH2	TIP	W	122	11.912	66.582	33.458	1.00	45.24	W
ATOM	1274	OH2	TIP	W	123	7.712	69.520	31.053	1.00	89.81	W
ATOM	1275	OH2	TIP	W	124	0.300	66.328	28.053	1.00	83.63	W
ATOM	1276	OH2	TIP	W	125	18.739	12.093	36.575	1.00	68.16	W
ATOM	1277	OH2	TIP	W	126	8.341	17.901	23.874	1.00	69.12	W
ATOM	1278	OH2	TIP	W	127	6.665	20.667	30.766	1.00	79.31	W
ATOM	1279	OH2	TIP	W	128	13.178	21.216	32.239	1.00	55.97	W
ATOM	1280	OH2	TIP	W	129	7.700	21.187	21.255	1.00	66.56	W
ATOM	1281	OH2	TIP	W	130	17.038	26.024	19.828	1.00	40.17	W
ATOM	1282	OH2	TIP	W	131	9.682	31.384	16.376	1.00	77.12	W
ATOM	1283	OH2	TIP	W	132	11.568	29.117	15.187	1.00	59.43	W
ATOM	1284	OH2	TIP	W	133	2.602	30.287	27.387	1.00	64.52	W
ATOM	1285	OH2	TIP	W	134	10.743	41.812	16.813	1.00	84.35	W
ATOM	1286	OH2	TIP	W	135	13.070	38.706	12.664	1.00	61.24	W
ATOM	1287	OH2	TIP	W	136	9.262	44.518	14.939	1.00	51.92	W
ATOM	1288	OH2	TIP	W	137	12.139	53.137	17.554	1.00	56.22	W
ATOM	1289	OH2	TIP	W	138	14.403	57.453	15.838	1.00	66.72	W
ATOM	1290	OH2	TIP	W	139	11.017	71.433	23.035	1.00	71.76	W
ATOM	1291	OH2	TIP	W	140	10.451	75.718	24.795	1.00	58.85	W
ATOM	1292	OH2	TIP	W	141	11.223	65.048	21.172	1.00	84.46	W
ATOM	1293	OH2	TIP	W	142	8.196	70.691	21.387	1.00	66.14	W
ATOM	1294	OH2	TIP	W	143	3.381	51.168	17.717	1.00	51.91	W
ATOM	1295	OH2	TIP	W	144	13.735	48.059	19.325	1.00	73.18	W
ATOM	1296	OH2	TIP	W	145	2.524	42.027	17.393	1.00	80.66	W
ATOM	1297	OH2	TIP	W	146	2.024	39.150	18.549	1.00	74.07	W
ATOM	1298	OH2	TIP	W	147	0.486	41.584	19.991	1.00	97.41	W
ATOM	1299	OH2	TIP	W	148	0.060	40.945	24.577	1.00	78.10	W
ATOM	1300	OH2	TIP	W	149	14.261	36.624	16.034	1.00	71.76	W
ATOM	1301	OH2	TIP	W	150	17.041	33.288	18.134	1.00	55.41	W
ATOM	1302	OH2	TIP	W	151	12.012	53.850	23.650	1.00	34.32	W
ATOM	1303	OH2	TIP	W	152	0.421	41.869	28.444	1.00	53.88	W
ATOM	1304	CL-1	CL	I	1	13.184	36.734	27.569	1.00	62.34	I
END											

Figure 11V